Clifford Algebras and Geometry of Entanglement

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ABSTRACT

In this thesis, the complex Clifford algebra and its representation are introduced as a foundation of our geometrical description of quantum states. An inner product and a metric are defined on the matrix representation in a natural way, so that it has the structure of a Hilbert space and a Riemannian manifold. In particular, the set of $D \times D$ pure density operators which describe n-qubit pure states, where $D = 2^n$ and n is a natural number, is characterised as the set of $D \times D$ positive operators whose associated quadratic forms satisfy the Fierz identities and the normalisation condition. Then this set is, in fact, nothing but the complex projective space $\mathbb{CP}^{D-1}$. Furthermore, the fibre bundle $S^{2D-1} \to \mathbb{CP}^{D-1}$ is derived from the construction of the space of $D \times D$ pure density operators, and its bundle projection provides the natural correspondence between the two formulations of quantum mechanics, namely, the state vector formulation and the density operator formulation.

The single qubit state case and the two-qubit pure state case are explored intensively as examples. For the single qubit case, both pure and mixed states are discussed explicitly in terms of the Clifford algebra description along with the 'mixedness' of a single qubit state, and the Riemannian structure of the space of single qubit pure density operators is examined. For the two-qubit case, the Clifford algebra description is discussed explicitly in relation to the Fierz identities, and, by employing the reduced density operators, it is shown that the concurrence of a two-qubit pure density operator coincides with the 'mixedness' of the reduced density operators. In addition, from this viewpoint, the "EPR paradox" is examined as a more geometrically precise illustrated example.

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Contents

1 Introduction

1.1 Historical background

Since the birth of quantum mechanics at the beginning of the 20th century, the behaviour of systems exhibiting "entanglement" has puzzled many physicists, and increasingly many people have realised its significance. Although more and more scientists have been involved in research on entanglement, there remains much scope for further investigation.

However, during the first half of the last century, only a few physicists seem to have pointed out the importance of the concept of "entanglement". It would be fair to say that one of the first notable milestones of entanglement was set in 1935, by Einstein, Podolsky and Rosen (EPR). Interestingly, their remarkable thought experiment called the "EPR paradox" was developed not to reveal the significance of entanglement but to demonstrate what they felt was a lack of completeness in quantum mechanics.

They strongly believed that Heisenberg's uncertainty principle, which is a key idea of quantum mechanics and claims that it is impossible to measure simultaneously both the position and the momentum of a particle with certainty, is a symbolic consequence of the incompleteness of quantum mechanics.

The logic of Einstein, Podolsky and Rosen was as follows. Suppose that two particles are in the entangled state

$$|\mathcal{B}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B \right),$$

(known as the Bell state or EPR pair[1]), where they could be light years apart, and Alice makes a measurement on the first particle and Bob on the second particle. If only one of them measures his or her own particle, its measurement outcome will be, say, either 0 or 1 with 50% probability. However, if one of them, say Alice, makes a measurement first, and after a short while Bob performs a measurement, then, surprisingly, Bob's measurement outcome seems to be affected by Alice's outcome. Namely, Bob will have exactly the same outcome as Alice without fail. Thus it seems that Bob's information, which says that his outcome is 0 (or 1), can be transmitted faster than the speed of light. On the other hand, Einstein had previously developed the theory of relativity, which says that nothing can travel faster

[1] We will see the rigorous definition for this object later in the thesis.

than the speed of light, and thus it clearly contradicts the above puzzling consequence. Therefore Einstein, Podolsky and Rosen claimed that, if we do not abandon relativity, it leads us to conclude that the quantum description of the two systems is incomplete, and there must be a "hidden-variable" to allow us to go beyond the uncertainty principle.

Note that the original "EPR paradox" was discussed in the context of continuous variable systems (for example, using eigenstates of position and momentum) whereas the above description assumes finite-dimensional state spaces. The transcription to the finite-dimensional case was carried out by Bohm in the 1950s.

This controversy had remained for many years until Bell proposed an experimental test, in 1964, which would be able to invalidate a local hidden-variable hypothesis. He found various inequalities which joint measurement probabilities would satisfy if hidden variables existed, and showed that two entangled quantum systems would violate these inequalities.

Here we are not going into the details of the Bell inequalities but the important point is that, contrary to Einstein's belief, quantum mechanics can violate these inequalities. Thus there can not exist any "hidden-variable", and this has been confirmed by experimental observations with many systems over last 30 years or so, especially in the work of Aspect.

However, we must note that this violation of the Bell inequalities does not ruin the credentials of the theory of relativity since, in the "EPR paradox", Alice still has to send Bob her measurement outcome via a classical channel, which does not involve travelling faster than the speed of light.

For more details, see a general reference on quantum mechanics [17], and references on the "EPR paradox" [8], [16] and [22].

1.2 Geometrical aspects of quantum entanglement

Over the last decade, a significant number of physicists, in their books and papers, have dealt with geometrical aspects of entanglement. Some of them successfully described the spaces of quantum pure states as the Hopf bundles ([15], [2] and [12]), whereas others provided extraordinarily concrete explanations regarding the spaces of quantum pure states as the complex projective spaces ([3], [24]).

More precisely, Mosseri and Dandoloff, in their paper [15], used the first Hopf bundle $S^3 \to S^2$ with complex numbers, and the second Hopf bundle $S^7 \to S^4$ with quaternions, to describe the geometry of single qubit states and two-qubit pure states, respectively (see Appendix B for more details). Their results, together with the generalization to three qubits [2], seemed to suggest that we could have much better understanding of the geometry of entanglement by employing this fibre bundle description for n-qubit pure states. However, there is a significant difficulty in applying this idea for the higher dimensional cases, since it is well-known that there are only three Hopf bundles, namely, $S^3 \to S^2$, $S^7 \to S^4$ and $S^{15} \to S^8$.

Moreover this Hopf bundle description was developed in terms of differential geometry by Lévay [12]. In particular, for the two-qubit pure state case, he described the second Hopf bundle $S^7 \to S^4$ by regarding S^4 as the quaternionic projective space $\mathbb{HP}^1$ endowed with the quaternionic generalisation of the Fubini-Study metric.

On the other hand, Brody and Hughston [3], and Życzkowski and Bengtsson [24] considered the spaces of quantum pure states as the complex projective spaces $\mathbb{CP}^m$, and described quantum entanglement in relation to projective geometry (or algebraic geometry in a broader sense). One of advantages of this approach seems to be that, unlike the Hopf bundle description, it can be applied to any n-qubit pure states, even though, in this case, the geometry of quantum states becomes more complicated than the Hopf bundle case. In addition, the formulations of quantum mechanics are based on the concept of complex Hilbert spaces. Therefore it seems to be more natural to consider geometry of quantum states in terms of complex geometry than to take 'quaternionic' geometry into account.

For these reasons, in this thesis we adopt the latter approach, namely the $\mathbb{CP}^m$ idea, even though we provide little rigorous discussion from the viewpoint of algebraic geometry.

Moreover there is another key concept which we embrace in this thesis. Some physicists, such as Dietz [6], employed the Clifford algebras as a platform for their discussion on quantum entanglement by 'embedding' quantum states in the algebras. This approach seems promising since an analogous discussion was successfully made, by Crawford [5], in the context of Dirac spinors along with the complex Clifford algebras, which may be another justification for our choice of the the $\mathbb{CP}^m$ view. In fact, in this thesis, many of the ideas in Crawford's paper are taken up and rewritten in suitable styles for our context.

1.3 Organisation

The organisation of this thesis is as follows.

In Chapter 2, we review the two formulations of quantum mechanics: the state vector formulation and the density operator formulation together with some basic definitions for quantum states. Then we describe the "EPR paradox" in terms of these formulations.

In Chapter 3, firstly we introduce the real Clifford algebra $Cl_N(\mathbb{R})$, where $N = 2n$ and n is an arbitrary natural number, and its matrix representation. Then we complexify the algebra to obtain the complex Clifford algebra $Cl_N(\mathbb{C})$, and also construct a Hermitian basis for its matrix representation $Mat(D, \mathbb{C})$, which is the matrix algebra of all $D \times D$ matrices, where $D = 2^n$.

In Chapter 4, an inner product and a metric are defined on the matrix representation $Mat(D, \mathbb{C})$ of $Cl_N(\mathbb{C})$, so that it obtains structures of a complex Hilbert space and a Riemannian manifold simultaneously. Then we discuss the space $\mathcal{Q}_D$ of all $D \times D$ pure density operators in relation to the Fierz identities and the fibre bundle $S^{2D-1} \longrightarrow \mathbb{CP}^{D-1}$. Lastly we show that the fibre bundle projection $h : S^{2D-1} \longrightarrow \mathbb{CP}^{D-1}$ is in fact the natural correspondence between the two formulations of quantum mechanics.

In Chapter 5, we concentrate on the single qubit case, including both the pure and mixed state case, as the most simple example of our Clifford algebra description of quantum states. We discuss the single qubit case explicitly alongside the first Hopf bundle $S^3 \longrightarrow S^2$, and introduce a measurement for 'mixedness' of a single qubit state. Also we show that the space $\mathcal{Q}_2$ of all 2×2 pure density operators is naturally identified with the complex projective space $\mathbb{CP}^1$ as a Riemannian manifold.

In Chapter 6, we focus on the two-qubit pure state case. We give an explicit description of two-qubit pure states in relation to the Fierz identities and the reduced density operators. Also, we revisit the "EPR paradox" to describe it geometrically in terms of our Clifford algebra formulation.

In Chapter 7, we give a summary of our discussion as a concluding chapter, together with several suggestions for possible further investigations.

In addition, we provide the following three Appendices.

In Appendix A, we introduce the definition and several geometrical properties of the complex projective space $\mathbb{CP}^m$, which plays a crucial role in this thesis.

In Appendix B, we give a short summary of the Hopf bundle description for single qubit and two-qubit pure states presented by Mosseri and Dandoloff [15] to contrast it with our Clifford algebra description.

In Appendix C, we show the details of the calculation to find 9 Fierz identities for the two-qubit pure state case.

In this thesis, we assume that the reader is familiar with Dirac notation for quantum states, and also with basic formal properties of complex inner product spaces (the assumption of completeness is not needed in what follows as we deal with only finite-dimensional spaces[2]), topology and differential geometry. Geometrical definitions will be provided as they arise in the constructions; general references on topology, differential geometry, complex manifolds and fibre bundles are [18], [7], [9], [20], [10] and [21].

Lastly, note that, in this thesis, we adopt both Dirac ket notation $|\psi\rangle$ and the usual notation ψ for vectors, and use either of them depending on the situation. In principle, Dirac notation is chosen when the context of the discussion is restricted to quantum states, and the usual notation is employed for more general cases.

[2]Every finite dimensional normed space is complete (for example, see [11]). Therefore every finite dimensional inner product space is complete, namely it is a Hilbert space.

2 Quantum mechanics and its postulates

In the first section of this chapter, we review the two formulations of quantum mechanics, namely the state vector formulation and the density operator formulation, providing some basic definitions for quantum states. In the next section, we revisit the "EPR paradox" as an example, which was introduced in the introduction, and describe it in the languages of these formulations.

2.1 State vector formulation and density operator formulation

The formulation of quantum mechanics is described mathematically by either state vectors or density operators (matrices), and it turns out that the two formulations are mathematically equivalent. Here we introduce both of the formulations and, later in Chapter 4, we see in what way these two formulations are linked.

To begin with, let us have a look at the state vector formulation along with the key postulates. The following presentation of the postulates of quantum mechanics is standard in many texts (see, for example, Sakurai [17]; we adopt the material from Nielsen and Chuang [16]).

Postulate 1: Associated to any isolated physical system is a complex vector space with inner product (that is, a Hilbert space) known as the ***state space*** of the system. The system is completely described by its ***state vector***, which is a unit vector in the system's state space.

Postulate 2: The evolution of a *closed* quantum system is described by a *unitary transformation*. That is, the state $|\psi\rangle$ of the system at time t_1 is related to the state $|\psi'\rangle$ of the system at time t_2 by a unitary operator U which depends only on the time t_1 and t_2,

$$|\psi'\rangle = U|\psi\rangle.$$

Postulate 3: Quantum measurements are described by a collection M_m of ***measurement operators***. These are operators acting on the state space of the system being measured. The index m refers to the measurement outcomes that may occur in the experiment. If the state of the quantum system is $|\psi\rangle$ immediately before the measurement, then the probability that result m occurs is given by

$$p(m) = \langle\psi|{M_m}^\dagger M_m|\psi\rangle,$$

and the state of the system after the measurement is

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|{M_m}^\dagger M_m|\psi\rangle}}.$$

The measurement operators satisfy the *completeness equation*,

$$\sum_m {M_m}^\dagger M_m = I.$$

Postulate 4: The state space of a composite physical system is the tensor product of the state space of the component physical systems. Moreover, if we have systems numbered 1 through k, and system number i is prepared in the state $|\psi_i\rangle$, then the joint state of the total system is $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_k\rangle$.

Remark. The matrix ${M_m}^\dagger M_m$ becomes positive, and this guarantees that the probability $p(m)$ is non-negative. To confirm this, put $|\varphi\rangle \equiv M_m|\psi\rangle$. Then

$$p(m) = \langle\psi|{M_m}^\dagger M_m|\psi\rangle = \langle\varphi|\varphi\rangle \geq 0.$$

Furthermore the completeness equation expresses the fact that probabilities sum to one:

$$\sum_m p(m) = \sum_m \langle\psi|{M_m}^\dagger M_m|\psi\rangle = \langle\psi|I|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

Now we turn to the density operator version of the story (Nielson and Chuang [16]).

Definition 2.1. Suppose that a quantum system is one of a number of states $|\psi_i\rangle$, where i is an index, with respective probabilities p_i. We shall call $\{p_i, |\psi_i\rangle\}$ an *ensemble of pure states.* The ***density operator (matrix)*** ρ for the system is defined by the equation

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|.$$

Remark. Importantly, it turns out that an operator ρ becomes the density operator associated with some ensemble $\{p_i, |\psi_i\rangle\}$ if and only if it is a positive operator with a unit trace [16]. This means that we could alternatively define a density as a positive operator with trace one. Also note that the density operator ρ is Hermitian since every positive operator is Hermitian.

Then, analogously to the state vector version, we have the following four postulates:

Postulate 1': Associated to any isolated physical system is a complex vector space with inner product (that is, a Hilbert space) known as the *state space* of the system. The system is completely described by its *density operator*, which is a *positive operator ρ with trace one*, acting on the state space of the system. If a quantum system is in the state ϱ_i with probability p_i, then the density operator for the system is $\sum_i p_i \varrho_i$.

Postulate 2': The evolution of a *closed* quantum system is described by a *unitary transformation*. That is, the state ρ of the system at time t_1 is related to the state ρ' of the system at time t_2 by a unitary operator U which depends only on the time t_1 and t_2,

$$\rho' = U \rho U^{\dagger}.$$

Postulate 3': Quantum measurements are described by a collection M_m of *measurement operators*. These are operators acting on the state space of the system being measured. The index m refers to the measurement outcomes that may occur in the experiments. If the state of the quantum system is ρ immediately before the measurement, then the probability that result m occurs is given by

$$p(m) = tr({M_m}^{\dagger} M_m \rho),$$

and the state of the system after the measurement is

$$\frac{M_m \rho {M_m}^{\dagger}}{tr({M_m}^{\dagger} M_m \rho)}.$$

The measurement operators satisfy the *completeness equation*,

$$\sum_m {M_m}^{\dagger} M_m = I.$$

Postulate 4': The state space of a composite physical system is the tensor product of the state space of the component physical systems. Moreover, if we have systems numbered 1 through k, and system number i is prepared in the state ϱ_i, then the joint state of the total system is $\varrho_1 \otimes \varrho_2 \otimes \cdots \otimes \varrho_k$.

Definition 2.2. A quantum system whose state $|\psi\rangle$ is known exactly is said to be in a ***pure state***. In this case the density operator is simply $\rho = |\psi\rangle\langle\psi|$. Otherwise, ρ is said to be in a ***mixed state***; it is said to be a mixture of the different pure states in the ensemble for ρ.

Remark. Clearly, ρ is in a pure state if and only if $rank(\rho) = 1$. This fact will be used frequently later in this thesis.

In addition, we have the following useful theorem and its corollary.

Theorem 2.1. *Let ρ be an arbitrary $n\times n$ non-zero positive operator. Then, $tr(\rho^2) \leq (tr(\rho))^2$, with equality if and only if there exists an n-dimensional complex vector $|\psi\rangle$ such that $\rho = |\psi\rangle\langle\psi|$.*

Proof. Since ρ is positive, we can assume that, with an appropriate orthonormal basis $\{|\psi_i\rangle\}$ for the state space,

$$\rho = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|,$$

where $p_i \geq 0$. Therefore, by applying $\langle\psi_i|\psi_j\rangle = \delta_{ij}$,

$$\rho^2 = \sum_{i,j=1}^{n} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| = \sum_{i=1}^{n} {p_i}^2 |\psi_i\rangle\langle\psi_i|.$$

Then, by the condition $p_i \geq 0$ and the triangle inequality,

$$tr(\rho^2) = \sum_{i=1}^{n} {p_i}^2 \leq \left(\sum_{i=1}^{n} p_i\right)^2 = (tr(\rho))^2.$$

Now, if there exists an n-dimensional complex vector $|\psi\rangle$ such that $\rho = |\psi\rangle\langle\psi|$, then we can define $|\psi_1\rangle \equiv |\psi\rangle/\sqrt{\langle\psi|\psi\rangle}$ and add other $(n-1)$ unit vectors to make up an orthonormal basis $\{|\psi_i\rangle\}$, which means that $p_1 = \langle\psi|\psi\rangle$ and $p_j = 0$ for $2 \leq j \leq n$. Therefore

$$tr(\rho^2) = {p_1}^2 = \langle\psi|\psi\rangle^2.$$

However

$$tr(\rho) = tr(|\psi\rangle\langle\psi|) = \langle\psi|\psi\rangle.$$

Hence

$$tr(\rho^2) = (tr(\rho))^2.$$

Conversely, if $tr(\rho^2) = (tr(\rho))^2$, then

$$\sum_{i=1}^{n} {p_i}^2 = \left(\sum_{i=1}^{n} p_i\right)^2. \tag{2.1}$$

To satisfy this equality, there needs to be exactly one index j such that $p_j > 0$ with the other p_i's being zero. In fact, if $p_j > 0$ and $p_k > 0$ with $j \neq k$, then

$$\sum_{i=1}^{n} {p_i}^2 < \sum_{i=1}^{n} {p_i}^2 + 2p_j p_k \leq \left(\sum_{i=1}^{n} p_i\right)^2.$$

Therefore the above equality (2.1) can not be satisfied. Moreover, for the above single index j,

$$\rho = p_j|\psi_j\rangle\langle\psi_j| = \left(\sqrt{p_j}|\psi_j\rangle\right)\left(\sqrt{p_j}\langle\psi_j|\right) \equiv |\psi\rangle\langle\psi|.$$

Hence the theorem is proved. $\square$

Corollary 2.2. *Let ρ be an $n \times n$ density operator. Then, $tr(\rho^2) \leq 1$, with equality if and only if ρ is a pure state. Alternatively, $tr(\rho^2) < 1$ if and only if ρ is in a mixed state.*

Proof. Obvious from the condition $tr(\rho) = 1$, Definition 2.2 and Theorem 2.1. $\square$

We now introduce more explicit definitions for single qubit pure states and two-qubit pure states.

Definition 2.3. Let $\mathcal{E}$ be a 2-dimensional Hilbert space over $\mathbb{C}$ (called a ***state space***), with an orthonormal basis $\{|0\rangle, |1\rangle\}$. A ***single qubit pure state (vector)*** for the state space $\mathcal{E}$ is defined as a unit vector $|\psi\rangle$ in $\mathcal{E}$ such that

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \qquad \alpha, \beta \in \mathbb{C} \text{ and } |\alpha|^2 + |\beta|^2 = 1. \tag{2.2}$$

Remark. We may rewrite the equation (2.2) as

$$|\psi\rangle = e^{i\chi}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right), \tag{2.3}$$

where $\chi, \varphi \in [0, 2\pi)$ and $\theta \in [0, \pi)$. Then, we see that the factor $e^{i\chi}$ can be ignored because it has no observable effects. Consequently, the equation can be simplified to

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle. \tag{2.4}$$

Therefore, $|\psi\rangle$ actually represents a point on S^2, and this sphere is called the ***Bloch sphere***.

Definition 2.4. Let $\mathcal{E}_1$ and $\mathcal{E}_2$ be 2-dimensional Hilbert spaces over $\mathbb{C}$ and let $\{|0\rangle_1, |1\rangle_1\}$ and $\{|0\rangle_2, |1\rangle_2\}$ be their orthonormal bases, respectively. Then,

$$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}, \qquad (\text{where } |ij\rangle \equiv |i\rangle_1 \otimes |j\rangle_2 \textit{ and } i, j \in \{0, 1\}),$$

becomes an orthonormal basis for the tensor product $\mathcal{E}_1 \otimes \mathcal{E}_2$ (called the ***composite state space***) of the Hilbert spaces $\mathcal{E}_1$ and $\mathcal{E}_2$. Now, a ***two-qubit pure state (vector)*** for the state space $\mathcal{E}_1 \otimes \mathcal{E}_2$ is defined as a unit vector $|\psi\rangle$ in $\mathcal{E}_1 \otimes \mathcal{E}_2$ such that

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle, \tag{2.5}$$

with $\quad \alpha, \beta, \gamma, \delta \in \mathbb{C} \quad$ and $\quad |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1.$

In addition, $|\psi\rangle$ is said to be ***separable*** if, by choosing an appropriate basis, it can be written as a tensor product of two single qubit pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ (*i.e.* $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = (\alpha_1|0\rangle_1 + \beta_1|1\rangle_1) \otimes (\alpha_2|0\rangle_2 + \beta_2|1\rangle_2)$). Otherwise, $|\psi\rangle$ is said to be ***entangled***.

Proposition 2.3. *The following is satisfied:*

$$|\psi\rangle \text{ is separable} \iff \alpha\delta = \beta\gamma, \tag{2.6}$$

$$|\psi\rangle \text{ is entangled} \iff \alpha\delta \neq \beta\gamma. \tag{2.7}$$

Proof. If $|\psi\rangle$ is separable, then, in the above expression,

$$|\psi\rangle = \alpha_1\alpha_2|00\rangle + \alpha_1\beta_2|01\rangle + \alpha_2\beta_1|10\rangle + \beta_1\beta_2|11\rangle.$$

Therefore, equating it with the expression (2.5), we have

$$\alpha = \alpha_1\alpha_2, \qquad \beta = \alpha_1\beta_2, \qquad \gamma = \alpha_2\beta_1, \qquad \delta = \beta_1\beta_2.$$

Hence

$$\alpha\delta - \beta\gamma = (\alpha_1\alpha_2)(\beta_1\beta_2) - (\alpha_1\beta_2)(\alpha_2\beta_1) = 0.$$

Conversely suppose that $\alpha\delta = \beta\gamma$. Since this identity is equivalent to $\alpha : \beta = \gamma : \delta$, there exists $\kappa \in \mathbb{C}$ such that $\gamma = \kappa\alpha$ and $\delta = \kappa\beta$. Thus

$$\begin{aligned} |\psi\rangle &= \alpha|00\rangle + \beta|01\rangle + \kappa\alpha|10\rangle + \kappa\beta|11\rangle \\ &= (|0\rangle + \kappa|1\rangle)\alpha|0\rangle + (|0\rangle + \kappa|1\rangle)\beta|1\rangle \\ &= (|0\rangle + \kappa|1\rangle) \otimes (\alpha|0\rangle + \beta|1\rangle). \end{aligned}$$

Hence $|\psi\rangle$ is separable. □

2.2 Interpretation of the "EPR paradox" in terms of the formulations

Now let us revisit the "EPR paradox" to describe it in terms of the above formulations. Recall that the two particles are in the entangled state

$$|\mathcal{B}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

Obviously this is a pure state since $|\mathcal{B}\rangle$ is written in the form of the equation (2.5). Therefore the corresponding density operator becomes

$$\rho_{\mathcal{B}} = |\mathcal{B}\rangle\langle\mathcal{B}| = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|).$$

Suppose that Alice makes a measurement on the first qubit in either the $|0\rangle$ direction or $|1\rangle$ direction, but she can not do anything with the second qubit. (Remember that the second qubit is far away from her.) Therefore, in this way, her measurement operators $\{M_m\}_{m=0,1}$ will be

$$\{M_m\}_{m=0,1} = \{|m\rangle\langle m| \otimes I\}_{m=0,1} = \{|m0\rangle\langle m0| + |m1\rangle\langle m1|\}_{m=0,1},$$

so that

$$\begin{aligned} {M_m}^\dagger M_m &= (|m0\rangle\langle m0| + |m1\rangle\langle m1|)\,(|m0\rangle\langle m0| + |m1\rangle\langle m1|) \\ &= |m0\rangle\langle m0| + |m1\rangle\langle m1|. \end{aligned}$$

Then, if only Alice makes a measurement, the probability for having the outcome m (m=0 or 1) will be

$$\begin{aligned} p(m) &= \langle \mathcal{B}|{M_m}^\dagger M_m|\mathcal{B}\rangle \\ &= \frac{1}{\sqrt{2}}\,(\langle 00| + \langle 11|)\,(|m0\rangle\langle m0| + |m1\rangle\langle m1|)\,\frac{1}{\sqrt{2}}\,(|00\rangle + |11\rangle) \\ &= \frac{1}{2}\,(\langle 00|m0\rangle\langle m0|00\rangle + \langle 11|m1\rangle\langle m1|11\rangle) \\ &= \frac{1}{2}\langle mm|mm\rangle\langle mm|mm\rangle = \frac{1}{2}\langle mm|mm\rangle = \frac{1}{2}. \end{aligned}$$

This shows that Alice has an equal 50% probability to obtain each outcome.

By the same token, Bob's measurement operators $\{N_n\}_{n=0,1}$ will be

$$\{N_n\}_{n=0,1} = \{I \otimes |n\rangle\langle n|\}_{n=0,1} = \{|0n\rangle\langle 0n| + |1n\rangle\langle 1n|\}_{n=0,1},$$

so that

$${N_n}^\dagger N_n = |0n\rangle\langle 0n| + |1n\rangle\langle 1n|.$$

Then, in the absence of Alice's measurement, the probability for the outcome n will be

$$p(n) = \langle \mathcal{B}|{N_n}^\dagger N_n|\mathcal{B}\rangle = \frac{1}{2},$$

where n=0 or 1, and Bob also has an equal 50% chance for each outcome.

However, we have a completely different story if Alice makes a measurement first and Bob measures his shortly afterwards. In that case, Alice still has a fifty-fifty chance for each outcome but the story changes immediately after this point. Namely, the measurement done by Alice changes the state of the qubits. If Alice makes a measurement with the operator M_m obtaining the outcome m, then the new state will become

$$\begin{aligned} |\mathcal{B}'\rangle &= \frac{M_m|\mathcal{B}\rangle}{\sqrt{\langle \mathcal{B}|{M_m}^\dagger M_m|\mathcal{B}\rangle}} = \sqrt{2}(|m0\rangle\langle m0| + |m1\rangle\langle m1|)\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ &= |m0\rangle\langle m0|00\rangle + |m1\rangle\langle m1|11\rangle = |mm\rangle, \end{aligned}$$

so that the new density operator becomes

$$\rho_{\mathcal{B}}{}' = |mm\rangle\langle mm|.$$

Now let us suppose that Alice obtained the outcome 0, and therefore the new state became $|\mathcal{B}'\rangle = |00\rangle$. If Bob makes a measurement with N_0, then he obtains the outcome 0 with probability

$$p'(0) = \langle\mathcal{B}'|N_0{}^{\dagger}N_0|\mathcal{B}'\rangle = \langle 00|\left(|00\rangle\langle 00| + |10\rangle\langle 10|\right)|00\rangle = 1.$$

On the contrary, if he makes a measurement with N_1, then the probability becomes

$$p'(1) = \langle\mathcal{B}'|N_1{}^{\dagger}N_1|\mathcal{B}'\rangle = \langle 00|\left(|01\rangle\langle 01| + |11\rangle\langle 11|\right)|00\rangle = 0.$$

These results show that Bob will have the outcome 0 with certainty.

Similarly, it can be shown that, if Alice has the outcome 1, then Bob's outcome also becomes 1 without fail.

We later revisit the "EPR paradox" as an example for the geometrical description of quantum entanglement in terms of our Clifford algebra formulation.

3 Clifford algebras

In this chapter, we introduce the Clifford algebras and their matrix representations as a platform of our discussion on quantum states in an analogous way to Crawford's approach to Dirac spinors [5]. General references on Clifford algebras and spinors are [1] and [13].

In the beginning section of this chapter, the real Clifford algebra $Cl_N(\mathbb{R})$, where $N = 2n$ and n is an arbitrary natural number, and its matrix representation are introduced. In the next section, we extend our discussion to the complex Clifford algebra $Cl_N(\mathbb{C})$, and construct a preferable Hermitian basis for its matrix representation $Mat(D, \mathbb{C})$, which is the matrix algebra consisting of all $D \times D$ matrices, where $D = 2^n$.

3.1 Real Clifford algebra $Cl_N(\mathbb{R})$

Definition 3.1. Let V be an N=$2n$-dimensional real vector space with a Euclidean metric[3] g, invariant under the orthogonal group $O(N)$, given by $g = (\delta_{ij})$ with $i, j = 1, 2, \ldots, N$. Let $\{\gamma_k\}_{k=1,2,\ldots,N}$ be an orthonormal basis for V with respect to the metric g. The ***real Clifford algebra*** $Cl_N(\mathbb{R})$ is the real vector space endowed with an associative product, distributive with respect to addition, and spanned by the set of N vectors γ_k, a unit $\mathbb{I}$, and their products which satisfy

$$\gamma_k \gamma_l + \gamma_l \gamma_k = 2\delta_{kl}\mathbb{I}, \tag{3.1}$$

with $k, l = 1, 2, \ldots, N$.

Remark. **(1)** As a vector space, the Clifford algebra $Cl_N(\mathbb{R})$ has dimension 2^N (as shown below), and its basis may be completed by adding elements of the following form to the set $\{\mathbb{I}, \gamma_k\}$:

$$\widetilde{\gamma}_{k_1 k_2 \cdots k_{N-M}} \equiv \frac{1}{M!} \sum_{k_{N-M+1}, \ldots, k_N} \epsilon_{k_1 k_2 \cdots k_N} \gamma_{k_{N-M+1}} \gamma_{k_{N-M+2}} \cdots \gamma_{k_N}, \tag{3.2}$$

where $M = 2, 3, \ldots, N$.

Then a set of elements forming a basis for $Cl_N(\mathbb{R})$ may be chosen to be

$$\{\gamma_A\} \equiv \{\mathbb{I}, \gamma_k, \widetilde{\gamma}_{k_1 k_2 \cdots k_{N-2}}, \ldots, \widetilde{\gamma}_k, \widetilde{\gamma}\},$$

[3]Obviously, the Euclidean metric g is naturally identified with the Euclidean inner product $\langle\ ,\ \rangle$, and we have $\langle \gamma_i, \gamma_j \rangle = \delta_{ij}$.

where $\widetilde{\gamma} \equiv \widetilde{\gamma}_{k_1 k_2 \cdots k_{N-N}}$ (*i.e.* $M = N$). Note that, for each combination $(k_1, k_2, \dots, k_{N-M})$ of $(N-M)$ numbers, there are $(N-M)!$ permutations. If $j_1 j_2 \cdots j_{N-M}$ and $l_1 l_2 \cdots l_{N-M}$ are two different permutations for the combination $(k_1, k_2, \dots, k_{N-M})$, then $\widetilde{\gamma}_{j_1 j_2 \cdots j_{N-M}}$ and $\widetilde{\gamma}_{l_1 l_2 \cdots l_{N-M}}$ turn out to be equal up to a plus or minus sign. In other words, $\widetilde{\gamma}_{j_1 j_2 \cdots j_{N-M}}$ and $\widetilde{\gamma}_{l_1 l_2 \cdots l_{N-M}}$ are linearly dependent. Therefore only one permutation needs to be chosen for each combination $(k_1, k_2, \dots, k_{N-M})$. For example, if $N = 4$ and $M = 2$, then we have $\widetilde{\gamma}_{12} = -\widetilde{\gamma}_{21}$, so that they are linearly dependent, and only one of them, say $\widetilde{\gamma}_{12}$, needs to be chosen as a basis element. For this reason, the number of the basis elements, namely the dimension of $Cl_N(\mathbb{R})$, is

$$\binom{N}{0} + \binom{N}{1} + \cdots + \binom{N}{N} = 2^N.$$

(2) The Clifford algebra $Cl_N(\mathbb{R})$ may be represented faithfully by $D \times D$ matrices where $D = 2^n$ [13]. Suppose that, under such a representation $\tau : Cl_N(\mathbb{R}) \longrightarrow Mat(D, \mathbb{C})$, each basis element γ_A is represented by Γ_A (*i.e.* $\tau(\gamma_A) = \Gamma_A$). More precisely, suppose that Γ_k $(k = 1, 2, \dots, N)$ and $\widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-M}}$ are the representing matrices for the basis elements γ_k $(k = 1, 2, \dots, N)$ and $\widetilde{\gamma}_{k_1 k_2 \cdots k_{N-M}}$, respectively. From the definition (3.2), we have the following equation for the matrix $\widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-M}}$:

$$\widetilde{\Gamma}_{k_1 k_2 .. k_{N-M}} = \frac{1}{M!} \sum_{k_{N-M+1}, .., k_N} \epsilon_{k_1 k_2 \cdots k_N} \Gamma_{k_{N-M+1}} \Gamma_{k_{N-M+2}} \cdots \Gamma_{k_N}, \tag{3.3}$$

where $M = 2, 3, \dots, N$.

Then the set of matrices

$$\{\Gamma_A\} = \{I, \Gamma_k, \widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-2}}, \dots, \widetilde{\Gamma}_k, \widetilde{\Gamma}\},$$

where $\widetilde{\Gamma} \equiv \widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-N}}$ (*i.e.* $M = N$), forms a basis for the matrix representation $\tau(Cl_N(\mathbb{R}))$ of the Clifford algebra $Cl_N(\mathbb{R})$. Clearly the number of the matrices Γ_A is $2^N = D^2$.

(3) Note that, obviously, since Γ_k are the representing matrices for γ_k, we have the corresponding equation:

$$\Gamma_k \Gamma_l + \Gamma_l \Gamma_k = 2\delta_{kl} I, \tag{3.4}$$

with $k, l = 1, 2, \dots, N$.

Example 3.1. In the case of $Cl_2(\mathbb{R})$ (*i.e.* $N = 2$), the real vector space V is 2-dimensional, so that the generators of $Cl_2(\mathbb{R})$ are γ_1 and γ_2. Then, from the definition (3.2), only one basis element is obtained (for the case where $M = N = 2$), namely

$$\widetilde{\gamma} = \frac{1}{2}(\epsilon_{12}\gamma_1\gamma_2 + \epsilon_{21}\gamma_2\gamma_1) = \gamma_1\gamma_2.$$

Therefore the basis for $Cl_2(\mathbb{R})$ is $\{\mathbb{I}, \gamma_1, \gamma_2, \widetilde{\gamma}\}$, and we may choose the representing matrices as follows:

$$\begin{aligned}
\text{unit element } \mathbb{I} &\simeq \text{identity matrix } I, \\
\gamma_1 &\simeq \Gamma_1 \equiv \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
\gamma_2 &\simeq \Gamma_2 \equiv \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\
\widetilde{\gamma} = \gamma_1\gamma_2 &\simeq \widetilde{\Gamma} = \Gamma_1\Gamma_2 = \sigma_1\sigma_2 = i\sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.
\end{aligned}$$

Example 3.2. In the case of $Cl_4(\mathbb{R})$ (*i.e.* $N = 4$), the real vector space V is 4-dimensional, and the generators of the algebra are γ_1, γ_2, γ_3 and γ_4. Then, from the definition (3.2), we have 11 more basis elements as follows.

If $M = 2$, then $N - M = 2$, so that we may choose the following 6 elements:

$$\widetilde{\gamma}_{12} = \frac{1}{2}(\epsilon_{1234}\gamma_3\gamma_4 + \epsilon_{1243}\gamma_4\gamma_3) = \gamma_3\gamma_4.$$

Similarly,

$$\begin{aligned}
\widetilde{\gamma}_{13} &= -\gamma_2\gamma_4, \quad \widetilde{\gamma}_{14} = \gamma_2\gamma_3, \quad \widetilde{\gamma}_{23} = \gamma_1\gamma_4, \\
\widetilde{\gamma}_{24} &= -\gamma_1\gamma_3 \quad \text{and} \quad \widetilde{\gamma}_{34} = \gamma_1\gamma_2.
\end{aligned}$$

If $M = 3$, then $N - M = 1$, and the following 4 elements may be chosen:

$$\begin{aligned}
\widetilde{\gamma}_1 &= \frac{1}{6}(\epsilon_{1234}\gamma_2\gamma_3\gamma_4 + \epsilon_{1243}\gamma_2\gamma_4\gamma_3 + \epsilon_{1324}\gamma_3\gamma_2\gamma_4 \\
&\quad + \epsilon_{1342}\gamma_3\gamma_4\gamma_2 + \epsilon_{1423}\gamma_4\gamma_2\gamma_3 + \epsilon_{1432}\gamma_4\gamma_3\gamma_2) \\
&= \gamma_2\gamma_3\gamma_4.
\end{aligned}$$

Similarly,

$$\widetilde{\gamma}_2 = -\gamma_1\gamma_3\gamma_4, \quad \widetilde{\gamma}_3 = \gamma_1\gamma_2\gamma_4, \quad \text{and} \quad \widetilde{\gamma}_4 = -\gamma_1\gamma_2\gamma_3.$$

If $M = 4$, then $N - M = 0$, so that only one basis element is obtained, that is

$$\begin{aligned}
\widetilde{\gamma} &= \frac{1}{24}(\epsilon_{1234}\gamma_1\gamma_2\gamma_3\gamma_4 + \epsilon_{1243}\gamma_1\gamma_2\gamma_4\gamma_3 + \cdots + \epsilon_{4321}\gamma_4\gamma_3\gamma_2\gamma_1) \\
&= \gamma_1\gamma_2\gamma_3\gamma_4.
\end{aligned}$$

Consequently, together with the unit element $\mathbb{I}$, the following 16 elements form a basis for $Cl_4(\mathbb{R})$:

$$\{\gamma_A\} = \{\mathbb{I}, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \widetilde{\gamma}_{12}, \widetilde{\gamma}_{13}, \widetilde{\gamma}_{14}, \widetilde{\gamma}_{23}, \widetilde{\gamma}_{24}, \widetilde{\gamma}_{34}, \widetilde{\gamma}_1, \widetilde{\gamma}_2, \widetilde{\gamma}_3, \widetilde{\gamma}_4, \widetilde{\gamma}\}.$$

3.2 Complex Clifford algebra $Cl_N(\mathbb{C})$

Since our framework is concerned with complex Hilbert spaces, the ***complex Clifford algebra*** $Cl_N(\mathbb{C}) \cong \mathbb{C} \otimes Cl_N(\mathbb{R})$ is the one which is really needed. Even though the basis $\{\Gamma_A\}$ for $\tau(Cl_N(\mathbb{R}))$ could be also used as a basis for $Mat(D, \mathbb{C})$ by allowing complex coefficients, a slight modification of the basis is required to adjust it to the density operator formulation.

To find an appropriate basis for $Mat(D, \mathbb{C})$, let us stick to the basis $\{\Gamma_A\}$ of $\tau(Cl_N(\mathbb{R}))$ for a little while. Now recall the definitions and the postulates of the density operator description. Since any density operator is Hermitian and any operator of the form $M^\dagger M$ is also Hermitian (they are actually both positive, and positive matrices are Hermitian), any such operator can be expressed as a linear combination with real coefficients in terms of an orthonormal Hermitian basis. More importantly, as we will see later in the thesis, such a Hermitian basis can be also employed as a basis for the D^2-dimensional real vector space $H(D, \mathbb{C})$ of all Hermitian matrices, where $H(D, \mathbb{C})$ is later formally defined as a subspace of $Mat(D, \mathbb{C})$ and plays a crucial role for our discussion. Therefore we require our expected basis for $Mat(D, \mathbb{C})$ to be Hermitian.

To construct the expected Hermitian basis for $Mat(D, \mathbb{C})$, we first prove the following lemma.

Lemma 3.1. *For every $k = 1, 2, \ldots, N$, let Γ_k be the representing matrix for the generator γ_k of $Cl_N(\mathbb{R})$ given in the last section. Then every Γ_k is Hermitian.*

Proof. It is well-known that any matrix in $Mat(D, \mathbb{C})$ has its Jordan canonical form. Therefore, for some $D \times D$ unitary matrix U,

$$\Gamma_k = U^\dagger \Lambda_k U,$$

where Λ_k is the Jordan canonical form of Γ_k. In addition, from the equation (3.4), we have ${\Gamma_k}^2 = I$, and this leads to

$${\Lambda_k}^2 = (U\Gamma_k U^\dagger)(U\Gamma_k U^\dagger) = U{\Gamma_k}^2 U^\dagger = UU^\dagger = I.$$

Thus the Jordan canonical form Λ_k is in fact diagonal. (It is easy to see that ${\Lambda_k}^2 = I$ is not satisfied if Λ_k is not diagonal.) Furthermore, since ${\Lambda_k}^2 = I$, each diagonal entry of Λ_k is either 1 or -1, so that ${\Lambda_k}^\dagger = \Lambda_k$. Therefore

$${\Gamma_k}^\dagger = U^\dagger \Lambda_k^\dagger U = U^\dagger \Lambda_k U = \Gamma_k.$$

Hence Γ_k is Hermitian. □

Now we are ready to define quadratic forms

$$\rho_0 \equiv \psi^\dagger \psi, \tag{3.5}$$

and

$$\rho_k \equiv \psi^\dagger \Gamma_k \psi, \tag{3.6}$$

where $k = 1, 2, \ldots, N$, and ψ is an arbitrary $D \times 1$ complex matrix (or vector). Here ψ does not need to be a unit vector to define the quadratic forms.

Note that our requirement for the matrices $\{\Gamma_A\}$ forces ρ_0 and ρ_k to be real. In fact, clearly, ρ_0 is real because it is $|\psi|^2$. In addition, for ρ_k, we see that

$$\rho_k = \psi^\dagger \Gamma_k \psi = \psi^\dagger {\Gamma_k}^\dagger \psi = \left(\psi^\dagger \Gamma_k \psi\right)^\dagger = \left(\psi^\dagger \Gamma_k \psi\right)^* = {\rho_k}^*,$$

where $k, = 1, 2, \ldots, N$, and ${\rho_k}^*$ denotes the complex conjugate of ρ_k.

Now let us consider the quadratic forms for the remaining Γ_A. From the equation (3.3), we have

$$(\psi^\dagger \widetilde{\Gamma}_{k_1 k_2 \ldots k_{N-M}} \psi)^* = (-1)^{\frac{1}{2}M(M-1)} \psi^\dagger \widetilde{\Gamma}_{k_1 k_2 \ldots k_{N-M}} \psi.$$

In fact,

$$\begin{aligned}
& (\psi^\dagger \widetilde{\Gamma}_{k_1 k_2 \ldots k_{N-M}} \psi)^* \\
= \; & (\psi^\dagger \widetilde{\Gamma}_{k_1 k_2 \ldots k_{N-M}} \psi)^\dagger \\
= \; & \psi^\dagger \left[\frac{1}{M!} \sum \epsilon_{k_1 k_2 \cdots k_N} \Gamma_{k_{N-M+1}} \Gamma_{k_{N-M+2}} \cdots \Gamma_{k_N} \right]^\dagger \psi \\
= \; & \psi^\dagger \left[\frac{1}{M!} \sum \epsilon_{k_1 k_2 \cdots k_N} (\Gamma_{k_N})^\dagger \cdots (\Gamma_{k_{N-M+2}})^\dagger (\Gamma_{k_{N-M+1}})^\dagger \right] \psi \\
= \; & \psi^\dagger \left[\frac{1}{M!} \sum \epsilon_{k_1 k_2 \cdots k_N} \Gamma_{k_N} \cdots \Gamma_{k_{N-M+2}} \Gamma_{k_N - M+1} \right] \psi \\
= \; & \psi^\dagger \left[\frac{1}{M!} \sum \epsilon_{k_1 k_2 \ldots k_N} \Gamma_{k_{N-M+1}} \Gamma_{k_{N-M+2}} \cdots \Gamma_{k_N} \cdot (-1)^{\frac{1}{2}M(M-1)} \right] \psi \\
= \; & (-1)^{\frac{1}{2}M(M-1)} \psi^\dagger \widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-M}} \psi.
\end{aligned}$$

Therefore the quadratic forms defined in this way would not be all real. Equivalently, the Γ_A are not all Hermitian. For this reason, we redefine the basis elements $\widetilde{\gamma}_{k_1 k_2 \ldots k_{N-M}}$ of the algebra $Cl_N(\mathbb{C})$ (and, automatically, the corresponding matrices $\widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}}$) as follows:

$$\widetilde{\gamma}_{k_1k_2\cdots k_{N-M}} \equiv i^{\frac{1}{2}M(M-1)}\frac{1}{M!}\sum_{k_{N-M+1},\ldots,k_N} \epsilon_{k_1k_2\cdots k_N}\gamma_{k_{N-M+1}}\cdots\gamma_{k_N}. \tag{3.7}$$

Remark. As mentioned, the above redefinition leads to the following equation:

$$\widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}} = i^{\frac{1}{2}M(M-1)}\frac{1}{M!}\sum_{k_{N-M+1},\ldots,k_N} \epsilon_{k_1k_2\cdots k_N}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}. \tag{3.8}$$

Definition 3.2. We define quadratic forms[4] ρ_A by

$$\rho_A \equiv \psi^\dagger\Gamma_A\psi \quad \text{for any } A, \tag{3.9}$$

where $\rho_0 \equiv \psi^\dagger I\psi = \psi^\dagger\psi$ and $\{\Gamma_A\} = \{I, \Gamma_k, \widetilde{\Gamma}_{k_1\cdots k_{N-2}}, \ldots, \widetilde{\Gamma}_k, \widetilde{\Gamma}\}$.

Remark. This definition is obviously consistent with the definition (3.5) and (3.6). Also note that ψ is not required to be a unit vector.

Then, we have the following proposition.

Proposition 3.2. *The following properties for the basis $\{\Gamma_A\}$ and the quadratic forms $\{\rho_A\}$ are satisfied:*

(1) *Every Γ_A is Hermitian.*

(2) *Every ρ_A is a real number.*

Proof. Since we have already had Lemma 3.1, it is sufficient to prove these claims for only the basis elements $\{\widetilde{\Gamma}_{k_1\cdots k_{N-M}}\}$ and the quadratic forms $\{\widetilde{\rho}_{k_1\cdots k_{N-M}}\}$, where the latter is defined by $\widetilde{\rho}_{k_1\cdots k_{N-M}} \equiv \psi^\dagger\widetilde{\Gamma}_{k_1\cdots k_{N-M}}\psi$.

[4]Strictly speaking, ρ_A is a quadratic form associated with a Hermitian form $\Omega_A(\varphi,\psi) = \varphi^\dagger\Gamma_A\psi$, so that we should denote it as $\rho_A(\psi) \equiv \psi^\dagger\Gamma_A\psi$ [14]. However we adopt the notation ρ_A for simplicity.

(1)

$$\begin{aligned}
&\left(\widetilde{\Gamma}_{k_1\ldots k_{N-M}}\right)^\dagger \\
=\ & \left[i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum_{k_{N-M+1},\cdots,k_N} \epsilon_{k_1k_2\ldots k_N} \Gamma_{k_{N-M+1}} \Gamma_{k_{N-M+2}} \cdots \Gamma_{k_N} \right]^\dagger \\
=\ & (i^*)^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1k_2\cdots k_N} (\Gamma_{k_N})^\dagger \cdots (\Gamma_{k_{N-M+2}})^\dagger (\Gamma_{k_{N-M+1}})^\dagger \\
=\ & (-i)^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1k_2\cdots k_N} \Gamma_{k_N} \cdots \Gamma_{k_{N-M+2}} \Gamma_{k_{N-M+1}} \\
=\ & (-i)^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1\cdots k_N} \Gamma_{k_N} \cdots \Gamma_{k_{N-M+1}} \cdot (-1)^{\frac{1}{2}M(M-1)} \\
=\ & \widetilde{\Gamma}_{k_1\cdots k_{N-M}}
\end{aligned}$$

Hence, every Γ_A is Hermitian.

(2)

$$\begin{aligned}
(\widetilde{\rho}_{k_1\cdots k_{N-M}})^* &= \left(\psi^\dagger \widetilde{\Gamma}_{k_1\cdots k_{N-M}} \psi\right)^* = \left(\psi^\dagger \widetilde{\Gamma}_{k_1\cdots k_{N-M}} \psi\right)^\dagger \\
&= \psi^\dagger (\widetilde{\Gamma}_{k_1\cdots k_{N-M}})^\dagger \psi = \psi^\dagger \widetilde{\Gamma}_{k_1\cdots k_{N-M}} \psi \\
&= \widetilde{\rho}_{k_1\cdots k_{N-M}}
\end{aligned}$$

Hence, every ρ_A is real.

□

We will see, in the next chapter, that the redefined matrix set $\{\Gamma_A\}$ is actually an orthonormal basis for $Mat(D, \mathbb{C})$ under a certain natural inner product, which we will call the Clifford algebra inner product. In fact, it turns out that, for even dimension N, $Cl_N(\mathbb{C})$ is isomorphic to $Mat(D, \mathbb{C})$ as an algebra [1], where $N = 2n$ and $D = 2^n$, so that the redefined matrix representation $\tau : Cl_N(\mathbb{C}) \longrightarrow Mat(D, \mathbb{C})$ becomes an algebra isomorphism.

Example 3.3. The basis for the complex Clifford algebra $Cl_2(\mathbb{C})$ is $\{\mathbb{I}, \gamma_1, \gamma_2, \widetilde{\gamma}\}$, and the representing matrix basis elements may be chosen as follows:

$$\begin{aligned}
\text{unit element } \mathbb{I} &\simeq \text{identity matrix } I, \\
\gamma_1 &\simeq \Gamma_1 \equiv \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\
\gamma_2 &\simeq \Gamma_2 \equiv \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
\widetilde{\gamma} = i\gamma_1\gamma_2 &\simeq \widetilde{\Gamma} = i\Gamma_1\Gamma_2 = i\sigma_1\sigma_2 = -\sigma_3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.
\end{aligned}$$

4 Clifford algebras and Quantum states

In this chapter, we develop our Clifford algebra description for quantum states in relation to the Fierz identities. Again, we adopt an analogous approach to Crawford's Dirac spinor version [5].

In the opening section of this chapter, we define an inner product and a metric on the matrix representation $\tau(Cl_N(\mathbb{C})) \cong Mat(D, \mathbb{C})$, where $N = 2n$, $D = 2^n$ and n is a natural number, so that it is ensured to be a complex Hilbert space and a Riemannian manifold simultaneously. Also the structure factors for the matrix representation are defined. In the following section, we derive the Fierz Identities, and show that they, together with the normalisation condition, characterise the space $\mathcal{Q_D}$ of all $D \times D$ pure density operators, where $D = 2^n$, in the sense that $\mathcal{Q_D}$ is identified with the space of all positive operators which define the quadratic forms which satisfy the Fierz identities and the normalisation condition. In the third section, we introduce the fibre bundle $S^{2D-1} \to \mathbb{CP}^{D-1}$, and see that the total space S^{2D-1} and the base space $\mathbb{CP}^{D-1}$ are in fact the space of all n-qubit pure state vectors and $\mathcal{Q_D}$, respectively. Then, in the last section, we show that the fibre bundle projection $h : S^{2D-1} \to \mathbb{CP}^{D-1}$ provides a natural correlation between the two formulations of quantum mechanics.

4.1 Clifford algebra inner product and Clifford algebra metric

For the basis matrices $\{\Gamma_A\}$ for the matrix representation $Mat(D, \mathbb{C})$ of the complex Clifford algebra $Cl_N(\mathbb{C})$, we have the following theorem.

Theorem 4.1.

(1) $(\Gamma_A)^2 = I$ *for any* Γ_A. *Therefore* $(\Gamma_A)^{-1} = \Gamma_A$ *and* $tr({\Gamma_A}^2) = D = 2^n$.

(2) *If* $\Gamma_A \neq I$, *then* $tr(\Gamma_A) = 0$.

(3) *If* $A \neq B$, *then* $tr(\Gamma_A \Gamma_B) = 0$.

Proof.

(1) If $\Gamma_A = I$ or Γ_k $(k = 1, 2, \ldots, N)$, clearly, the claim is satisfied because of the equation (3.4).

If $\Gamma_A = \widetilde{\Gamma}$,

$$\widetilde{\Gamma} = i^{\frac{1}{2}N(N-1)} \frac{1}{N!} \sum_{k_1,k_2,..,k_N} \epsilon_{k_1 k_2 \cdots k_N} \Gamma_{k_1} \Gamma_{k_2} \cdots \Gamma_{k_N}.$$

Applying the inverse permutation of indices to each of the $N!$ terms to recover the ordering $(1, 2, \ldots, N)$, we have

$$\widetilde{\Gamma} = i^{\frac{1}{2}N(N-1)} \frac{1}{N!} \sum_{k_1,..,k_N} (\epsilon_{k_1 \cdots k_N})^2 \Gamma_1 \Gamma_2 \cdots \Gamma_N = i^{\frac{1}{2}N(N-1)} \Gamma_1 \Gamma_2 \cdots \Gamma_N.$$

Then

$$\begin{aligned}
\left(\widetilde{\Gamma}\right)^2 &= \left[i^{\frac{1}{2}N(N-1)} \Gamma_1 \Gamma_2 \cdots \Gamma_N\right]^2 \\
&= (-1)^{\frac{1}{2}N(N-1)} (\Gamma_1 \Gamma_2 \cdots \Gamma_N)(\Gamma_1 \Gamma_2 \cdots \Gamma_N) \\
&= (-1)^{\frac{1}{2}N(N-1)} (\Gamma_1)^2 (\Gamma_2 \Gamma_3 \cdots \Gamma_N)(\Gamma_2 \Gamma_3 \cdots \Gamma_N) \cdot (-1)^{N-1} \\
&= (-1)^{\frac{1}{2}N(N-1)} (\Gamma_1)^2 (\Gamma_2)^2 \cdots (\Gamma_N)^2 \cdot (-1)^{\frac{1}{2}N(N-1)} \\
&= I.
\end{aligned}$$

Finally, suppose that $\Gamma_A = \widetilde{\Gamma}_{k_1 k_2 \ldots k_{N-M}}$, and let $l_{N-M+1}, l_{N-M+2}, .., l_N$ be a certain fixed ordering of the index set $\{k_{N-M+1}, k_{N-M+2}, \ldots k_N\}$. Also, for each ordering $k_{N-M+1}, k_{N-M+2}, \ldots k_N$, let π be the permutation of the index set such that

$$\pi(l_j) = k_j, \qquad \text{where } j = N - M + 1, N - M + 2, \ldots, N.$$

Then we have

$$\begin{aligned}
& \widetilde{\Gamma}_{k_1 \ldots k_{N-M}} \\
= \;& i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum_{k_{N-M+1},..,k_N} \epsilon_{k_1 \cdots k_N} \Gamma_{k_{N-M+1}} \Gamma_{k_{N-M+2}} \cdots \Gamma_{k_N} \\
= \;& i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1 \cdots k_N} \Gamma_{\pi(l_{N-M+1})} \cdots \Gamma_{\pi(l_N)} \\
= \;& i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1 \cdots k_N} sgn(\pi^{-1}) \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N} \\
= \;& i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1 \cdots k_{N-M} \pi^{-1}(k_{N-M+1}) \cdots \pi^{-1}(k_N)} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N} \\
= \;& i^{\frac{1}{2}M(M-1)} \frac{1}{M!} \sum \epsilon_{k_1 \cdots k_{N-M} l_{N-M+1} \cdots l_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N}.
\end{aligned}$$

Note that, in the last line, the term $\epsilon_{k_1 \cdots k_{N-M} l_{N-M+1} \cdots l_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N}$ is independent of the indices $k_{N-M+1}, .., k_N$, and the summation here is nothing but $M! \times \epsilon_{k_1 \cdots k_{N-M} l_{N-M+1} \cdots l_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N}$. Therefore

$$\widetilde{\Gamma}_{k_1 \ldots k_{N-M}} = i^{\frac{1}{2}M(M-1)} \epsilon_{k_1 \cdots k_{N-M} l_{N-M+1} \cdots l_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N}.$$

Consequently, similarly to the previous case,

$$
\begin{aligned}
&\left(\widetilde{\Gamma}_{k_1\ldots k_{N-M}}\right)^2 \\
= \ & (-1)^{\frac{1}{2}M(M-1)}(\epsilon_{k_1\cdots k_{N-M}l_{N-M+1}\cdots l_N})^2(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N})^2 \\
= \ & (-1)^{\frac{1}{2}M(M-1)}(\Gamma_{k_{N-M+1}})^2\cdots(\Gamma_{k_N})^2(-1)^{\frac{1}{2}M(M-1)} \\
= \ & I.
\end{aligned}
$$

(2) Firstly suppose that $\Gamma_A = \Gamma_k$ $(k = 1, 2, \cdots, N)$. Then for $l \neq k$, $(l = 1, 2, \cdots, N)$, the anti-symmetric condition $\Gamma_k\Gamma_l + \Gamma_l\Gamma_k = 0$ leads to

$$\Gamma_k = -\Gamma_l\Gamma_k{\Gamma_l}^{-1}.$$

thus

$$tr(\Gamma_k) = -tr(\Gamma_l\Gamma_k{\Gamma_l}^{-1}) = -tr({\Gamma_l}^{-1}\Gamma_l\Gamma_k) = -tr(\Gamma_k).$$

Hence

$$tr(\Gamma_k) = 0.$$

Next suppose that $\Gamma_A = \widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}}$. In this case, since

$$\widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}} = i^{\frac{1}{2}M(M-1)}\frac{1}{M!}\sum_{k_{N-M+1},\ldots,k_N}\epsilon_{k_1k_2\cdots k_N}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N},$$

in order to prove that $tr\left(\widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}}\right) = 0$, all that we need to show is

$$tr(\Gamma_{k_{N-M+1}}\Gamma_{k_{N-M+2}}\cdots\Gamma_{k_N}) = 0.$$

Now if M is even,

$$\Gamma_{k_{N-M+1}}\Gamma_{k_{N-M+2}}\cdots\Gamma_{k_N-1}\Gamma_{k_N} = -\Gamma_{k_N}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1},$$

but

$$
\begin{aligned}
tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}\Gamma_{k_N}) &= -tr(\Gamma_{k_N}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}) \\
&= -tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}\Gamma_{k_N}).
\end{aligned}
$$

Hence

$$tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}\Gamma_{k_N}) = 0.$$

If M is odd, there always exists a generator $\Gamma_{k_{N-M}}$ such that

$$\Gamma_{k_{N-M}} \notin \{\Gamma_{k_{N-M+1}}, \cdots, \Gamma_{k_N}\},$$

since we always have the even number of the generators in total. Therefore

$$\begin{aligned}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N} &= \Gamma_{k_{N-M}}\Gamma_{k_{N-M}}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}\\ &= -\Gamma_{k_{N-M}}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}\Gamma_{k_{N-M}}.\end{aligned}$$

Thus

$$\begin{aligned}tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}) &= -tr(\Gamma_{k_{N-M}}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N-1}\Gamma_{k_{N-M}})\\ &= -tr(\Gamma_{k_{N-M}}\Gamma_{k_{N-M}}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N})\\ &= -tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}).\end{aligned}$$

Hence

$$tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}) = 0.$$

Consequently, we have

$$tr\left(\widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}}\right) = 0.$$

(3) If $\Gamma_A = I$ or $\Gamma_B = I$, this statement becomes nothing but the above claim (2), which has been just proved.

If $\Gamma_A = \Gamma_k$ and $\Gamma_B = \Gamma_l$ with $k \neq l$ $(k, l = 1, 2, \ldots, N)$, then, from the equation (3.4),

$$\Gamma_k\Gamma_l + \Gamma_l\Gamma_k = 0$$

$$tr(\Gamma_k\Gamma_l + \Gamma_l\Gamma_k) = 0$$

$$tr(\Gamma_k\Gamma_l) = -tr(\Gamma_l\Gamma_k).$$

However, also

$$tr(\Gamma_k\Gamma_l) = tr(\Gamma_l\Gamma_k).$$

Hence

$$tr(\Gamma_k\Gamma_l) = 0.$$

Next, suppose that $\Gamma_A = \widetilde{\Gamma}_{k_1k_2\cdots k_{N-M}}$ and $\Gamma_B = \Gamma_l$ $(l = 1, 2, \ldots, N)$. Since

$$\widetilde{\Gamma}_{k_1k_2\ldots k_{N-M}} = i^{\frac{1}{2}M(M-1)}\frac{1}{M!}\sum_{k_{N-M+1},\ldots,k_N}\epsilon_{k_1k_2\cdots k_N}\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N},$$

again, it is sufficient to show that

$$tr(\Gamma_{k_{N-M+1}}\cdots\Gamma_{k_N}\Gamma_l) = 0.$$

However this can be shown in a similar manner to the above claim (2).

Lastly, suppose that $\Gamma_A = \widetilde{\Gamma}_{k_1 k_2 \cdots k_{N-M}}$ and $\Gamma_B = \widetilde{\Gamma}_{l_1 l_2 \cdots k_{N-L}}$ satisfying $\Gamma_A \neq \Gamma_B$. In this case, the equation (3.8) implies that we need to show that

$$tr(\Gamma_{k_{N-M+1}} \cdots \Gamma_{k_N} \Gamma_{l_{N-L+1}} \cdots \Gamma_{l_N}) = 0.$$

Since the two combinations $(k_1, k_2, \ldots, k_{N-M})$ and $(l_1, l_2, \ldots, l_{N-L})$ are different, evidently, it can never be satisfied that

$$\Gamma_{k_{N-M+1}} \cdots \Gamma_{k_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N} = cI,$$

where c is a constant. This means that $\Gamma_{k_{N-M+1}} \cdots \Gamma_{k_N} \Gamma_{l_{N-M+1}} \cdots \Gamma_{l_N}$ is, in any case, a product of some different Γ_k even though it is reduced to the simplest form. Therefore, again, similarly to the previous case (2), we see that

$$tr(\Gamma_{k_{N-M+1}} \cdots \Gamma_{k_N} \Gamma_{l_{N-L+1}} \cdots \Gamma_{l_N}) = 0.$$

Hence the claim is proved.

□

Definition 4.1. We define the ***Clifford algebra inner product*** $\langle\ ,\ \rangle_C$ and the ***Clifford algebra metric***[5] G_{IJ} as a natural inner product and a natural metric, respectively, on the matrix representation $\tau(Cl_N(\mathbb{C})) \cong Mat(D, \mathbb{C})$ given by

$$\langle \Gamma_I, \Gamma_J \rangle_C \equiv G_{IJ} \equiv \frac{1}{D} tr(\Gamma_I \Gamma_J), \tag{4.1}$$

where $\Gamma_I, \Gamma_J \in \{\Gamma_A\}$.

Remark. From Theorem 4.1, we see that $\langle \Gamma_I, \Gamma_J \rangle_C = G_{IJ} = \delta_{IJ}$, and the matrix (G_{IJ}) becomes the $2^N \times 2^N$ identity matrix I_{2^N}. In other words, under this inner product, the basis $\{\Gamma_A\}$ becomes an orthonormal basis. Furthermore, for any two $D \times D$ complex matrices ρ and σ, the inner product $\langle \rho, \sigma \rangle_C$ on $Mat(D, \mathbb{C})$ is given by

$$\langle \rho, \sigma \rangle_C = \frac{1}{D} tr(\rho \sigma). \tag{4.2}$$

Then the norm $\|\rho\|_C$ on $Mat(D, \mathbb{C})$ is naturally defined by

$$\|\rho\|_C \equiv \sqrt{\langle \rho, \rho \rangle_C} = \sqrt{\frac{1}{D} tr(\rho^2)}. \tag{4.3}$$

[5]Here we define an inner product and a metric simultaneously. This is possible since, like $\mathbb{R}^n$ or $\mathbb{C}^n$, $Mat(D, \mathbb{C})$ is naturally identified with its (co)tangent space at its origin together with its inner product [20]. Also, note that our Clifford algebra inner product (or metric) is nothing but the Hilbert-Schmidt inner product apart from the constant $1/D$ [16].

In addition, because of this ideal property, we have the following key theorem.

Theorem 4.2. *Let $\mathcal{E} \equiv \otimes_{i=1}^{n} \mathcal{E}_i$ be a composite Hilbert space of complex D=2^n-dimension, and let ρ be an arbitrary $D \times D$ operator. Then*

$$\rho = \frac{1}{D} \sum_I \omega_I \Gamma_I, \tag{4.4}$$

where $\omega_I = tr(\rho\Gamma_I)$ and $\Gamma_I \in \{\Gamma_A\}$.

Proof. Since $\{\Gamma_A\}$ is a basis for $Mat(D, \mathbb{C})$, ρ can be written as

$$\rho = \sum_J \alpha_J \Gamma_J,$$

where $\alpha_J \in \mathbb{C}$. Then, since $tr(\Gamma_J\Gamma_I) = D\delta_{JI}$,

$$\omega_I = tr(\rho\Gamma_I) = \sum_J \alpha_J tr(\Gamma_J\Gamma_I) = \alpha_I tr({\Gamma_I}^2) = D\alpha_I.$$

Thus

$$\alpha_I = \frac{1}{D}\omega_I.$$

Hence

$$\rho = \sum_J \alpha_J \Gamma_J = \sum_I \alpha_I \Gamma_I = \frac{1}{D} \sum_I \omega_I \Gamma_I.$$

□

Remark. Here, together with Corollary 4.3, we assume that ψ does not need to be a unit vector, and ρ does not need to be a density operator. Note that, since $\omega_I = tr(\rho\Gamma_I) = D\langle\rho, \Gamma_I\rangle_C$, the equation (4.4) becomes

$$\rho = \sum_I \langle\rho, \Gamma_I\rangle_C \Gamma_I, \tag{4.5}$$

which is one of the basic properties for inner product spaces. Also, for two arbitrary $D \times D$ operators $\rho = \frac{1}{D}\sum_I \omega_I \Gamma_I$ and $\sigma = \frac{1}{D}\sum_J \eta_J \Gamma_J$, where $\omega_I = tr(\rho\Gamma_I)$ and $\eta_J = tr(\sigma\Gamma_J)$,

$$\begin{aligned}
\langle\rho, \sigma\rangle_C &= \frac{1}{D} tr(\rho\sigma) = \frac{1}{D^3} \sum_{I,J} \omega_I \eta_J tr(\Gamma_I \Gamma_J) \\
&= \frac{1}{D^3} \sum_I \omega_I \eta_I tr({\Gamma_I}^2) = \frac{1}{D^3} \sum_I \omega_I \eta_I tr(I) \\
&= \frac{1}{D^2} \sum_I \omega_I \eta_I.
\end{aligned} \tag{4.6}$$

In particular, we have

$$\|\rho\|_C = \sqrt{\langle \rho, \rho \rangle_C} = \frac{1}{D}\sqrt{\sum_I \omega_I{}^2}. \tag{4.7}$$

Corollary 4.3. *Let $\mathcal{E} \equiv \otimes_{i=1}^n \mathcal{E}_i$ be a composite Hilbert space of complex dimension $D=2^n$, and let ρ be an arbitrary $D \times D$ operator. If there exists a vector $\psi \in \mathcal{E}$ such that $\rho = \psi\psi^\dagger$, then*

$$\rho = \frac{1}{D}\sum_I \rho_I \Gamma_I, \tag{4.8}$$

where $\rho_I = \psi^\dagger \Gamma_I \psi$ and $\Gamma_I \in \{\Gamma_A\}$.

Proof. By assumption,

$$\rho_I = \psi^\dagger \Gamma_I \psi = tr(\psi^\dagger \Gamma_I \psi) = tr(\psi\psi^\dagger \Gamma_I) = tr(\rho\Gamma_I) = \omega_I.$$

Then, by Theorem 4.2,

$$\rho = \frac{1}{D}\sum_I \rho_I \Gamma_I.$$

□

Remark. The assumption of Corollary 4.3 implies that the definition $\rho_I = \psi^\dagger \Gamma_I \psi$ can not be applied to mixed states since the existence of the vector ψ is not guaranteed. To avoid this inconvenience, we could alternatively define ρ_I by $\rho_I \equiv tr(\rho\Gamma_I)$. However we do not choose this way so that we can describe the fibre bundle structure of the n-qubit pure states in a more comprehensible way.

Definition 4.2. The ***structure factors*** C_{IJK} and C_{IJKL} for the matrix representation $Mat(D, \mathbb{C})$ of the Clifford algebra $Cl_N(\mathbb{C})$ are defined by

$$C_{IJK} \equiv \frac{1}{D} tr(\Gamma_I \Gamma_J \Gamma_K), \tag{4.9}$$

$$C_{IJKL} \equiv \frac{1}{D} tr(\Gamma_I \Gamma_J \Gamma_K \Gamma_L). \tag{4.10}$$

Remark. **(1)** Equivalently, the structure factors could be defined by the following equations:

$$\Gamma_I \Gamma_J = \sum_K C_{IJK} \Gamma_K, \tag{4.11}$$

$$\Gamma_I \Gamma_J \Gamma_K = \sum_L C_{IJKL} \Gamma_L. \tag{4.12}$$

In fact, if the equation (4.11) is satisfied, then

$$\Gamma_I\Gamma_J\Gamma_A = \left(\sum_K C_{IJK}\Gamma_K\right)\Gamma_A.$$

Then, taking the trace of each side, we have

$$\begin{aligned} tr(\Gamma_I\Gamma_J\Gamma_A) &= \sum_K C_{IJK}\, tr\,(\Gamma_K\Gamma_A) \\ &= \sum_K C_{IJK}\delta_{KA}\cdot D = C_{IJA}\cdot D. \end{aligned}$$

Hence

$$C_{IJA} = \frac{1}{D} tr(\Gamma_I\Gamma_J\Gamma_A).$$

Conversely suppose that we have the equation (4.9). Since $Mat(D,\mathbb{C})$ is closed under matrix multiplication, for any product $\Gamma_I\Gamma_J$, there exist complex numbers α_{IJK} such that

$$\Gamma_I\Gamma_J = \sum_K \alpha_{IJK}\Gamma_K.$$

Therefore

$$\Gamma_I\Gamma_J\Gamma_A = \left(\sum_K \alpha_{IJK}\Gamma_K\right)\Gamma_A,$$

so that

$$\begin{aligned} tr(\Gamma_I\Gamma_J\Gamma_A) &= \sum_K \alpha_{IJK}\, tr\,(\Gamma_K\Gamma_A) = \sum_K \alpha_{IJK}\delta_{KA}\cdot D \\ &= D\alpha_{IJK}. \end{aligned}$$

Thus

$$\alpha_{IJA} = \frac{1}{D} tr(\Gamma_I\Gamma_J\Gamma_A) = C_{IJA}.$$

Hence

$$\Gamma_I\Gamma_J = \sum_K C_{IJK}\Gamma_K.$$

Similarly we can see that the equation (4.10) and the equation (4.12) are equivalent.

(2) Clearly, from the above definition, both of these structure factors are invariant under cyclic permutation of their indices, that is,

$$C_{IJK} = C_{JKI} = C_{KIJ}, \tag{4.13}$$

and

$$C_{IJKL} = C_{JKLI} = C_{KLIJ} = C_{LIJK}. \tag{4.14}$$

4.2 The Fierz identities

Firstly let us define a new notation for the sake of convenience as noted earlier. We define $H(D, \mathbb{C})$ by

$$H(D, \mathbb{C}) \equiv \{X^\dagger = X \mid X \in Mat(D, \mathbb{C})\}.$$

(i.e. $H(D, \mathbb{C})$ is the set of all $D \times D$ Hermitian matrices.) Clearly, $H(D, \mathbb{C})$ becomes a D^2-dimensional vector space over $\mathbb{R}$, so that it may be regarded as a subspace of the $2D^2$-dimensional real vector space $Mat(D, \mathbb{C})$. In addition, the basis $\{\Gamma_A\}$ can be adopted as a basis for $H(D, \mathbb{C})$ allowing only real coefficients. However $H(D, \mathbb{C})$ cannot be an algebra since a product of two Hermitian matrices is not usually Hermitian.

Now let us consider the map

$$\begin{array}{rcccl} \widetilde{h}: \ \mathcal{E} \equiv \otimes_{i=1}^{n} \mathcal{E}_i & \longrightarrow & H(D, \mathbb{C}) & \subset & Mat(D, \mathbb{C}) \\ \psi & \longmapsto & \psi\psi^\dagger = \rho & & \end{array} , \tag{4.15}$$

where $N = 2n$, $D = 2^n$, ψ is an arbitrary vector in a composite Hilbert space $\mathcal{E}$, ρ is the corresponding Hermitian operator, $\rho_I = \psi^\dagger \Gamma_I \psi$ and $\Gamma_I \in \{\Gamma_A\}$. Note that, at this stage, we do not yet require either ψ to be a unit vector or ρ to be a density operator.

Now recall that ψ is a D-dimensional complex vector, so that it can be regarded as a $2D$-dimensional real vector. Also ρ can be regarded as a D^2-dimensional real vector since $\rho \in H(D, \mathbb{C})$.

However, even though ρ has D^2 real components, they are not all independent. In fact, as ρ is only composed of $2D$ real (or D complex) functions, and furthermore, as ρ is not affected by an overall phase factor $\psi \to e^{i\chi}\psi$, only $(2D-1)$ real components of ρ may be considered to be independent. In other words, among D^2 quadratic forms $\{\rho_A\}$, only $(2D-1)$ of them are independent. Therefore the quadratic forms must satisfy a system of $(D-1)^2$ independent equations, which are called the ***Fierz identities***.

Theorem 4.4. *(Fierz identities)*
Let $\mathcal{E} \equiv \otimes_{i=1}^{n} \mathcal{E}_i$ be a composite Hilbert space of complex dimension D=2^n, and suppose that ρ is an arbitrary operator in $H(D, \mathbb{C})$. If there exists a vector $\psi \in \mathcal{E}$ such that $\rho = \psi\psi^\dagger$, then

$$\rho_I \rho_J = \frac{1}{D} \sum_{K,L} C_{KILJ} \rho_K \rho_L, \tag{4.16}$$

where $\rho_A = \psi^\dagger \Gamma_A \psi$.

Proof.

$$\rho_I \rho_J = (\psi^\dagger \Gamma_I \psi)(\psi^\dagger \Gamma_J \psi) = \psi^\dagger \Gamma_I \rho \Gamma_J \psi.$$

Then, by Corollary 4.3 and the equation (4.12),

$$\begin{aligned}
\rho_I \rho_J &= \psi^\dagger \Gamma_I \left(\frac{1}{D} \sum_K \rho_K \Gamma_K \right) \Gamma_J \psi = \frac{1}{D} \sum_K \rho_K \psi^\dagger \left(\Gamma_I \Gamma_K \Gamma_J \right) \psi \\
&= \frac{1}{D} \rho_K \psi^\dagger \left(\sum_L C_{IKJL} \Gamma_L \right) \psi = \frac{1}{D} \sum_{K,L} C_{IKJL} \rho_K \psi^\dagger \Gamma_L \psi \\
&= \frac{1}{D} \sum_{K,L} C_{IKJL} \rho_K \rho_L.
\end{aligned}$$

□

Remark. Even though $\frac{1}{2}D^2(D^2+1)$ identities can be derived from the equation (4.16), only $(D-1)^2$ of them are independent due to the reason stated above.

What about the inverse proposition to Theorem 4.4? We prove that it is also the case.

Theorem 4.5. *Let $\mathcal{E} \equiv \otimes_{i=1}^n \mathcal{E}_i$ be a composite Hilbert space of complex D=2^n-dimension, and let ρ be an arbitrary positive operator in $H(D,\mathbb{C})$. If, for any ω_A defined by $\omega_A = tr(\rho\Gamma_A)$, the identities*

$$\omega_I \omega_J = \frac{1}{D} \sum_{K,L} C_{KILJ} \omega_K \omega_L, \tag{4.17}$$

are satisfied, then there exists a vector $\psi \in \mathcal{E}$ such that $\psi\psi^\dagger = \rho$.

Proof. From Theorem 4.2,

$$\rho = \frac{1}{D} \sum_A \omega_A \Gamma_A, \qquad \text{where } \omega = tr(\rho\Gamma_A).$$

Thus

$$\begin{aligned}
\rho \Gamma_I \rho &= \left(\frac{1}{D} \sum_K \omega_K \Gamma_K \right) \Gamma_I \left(\frac{1}{D} \sum_L \omega_L \Gamma_L \right) \\
&= \frac{1}{D^2} \sum_{K,L} \omega_K \omega_L \Gamma_K \Gamma_I \Gamma_L.
\end{aligned}$$

Then, from the equation (4.12) and (4.17),

$$
\begin{aligned}
\rho\Gamma_I\rho &= \frac{1}{D^2}\sum_{J,K,L}\omega_K\omega_L C_{KILJ}\Gamma_J \\
&= \frac{1}{D}\sum_J\left(\frac{1}{D}\sum_{K,L}C_{KILJ}\omega_K\omega_L\right)\Gamma_J \\
&= \frac{1}{D}\sum_J\omega_I\omega_J\Gamma_J \\
&= \omega_I\rho.
\end{aligned}
$$

In particular, if $\Gamma_I = I$, we have

$$\rho^2 = \omega_0\rho.$$

Thus

$$tr(\rho^2) = \omega_0 tr(\rho).$$

However, $\omega_0 = tr(\rho)$, so that

$$tr(\rho^2) = (tr(\rho))^2.$$

Hence, from Theorem 2.1, there exists a vector $\psi \in \mathcal{E}$ such that $\psi\psi^\dagger = \rho$. $\square$

Remark. Since the existence of such a vector ψ is guaranteed as a result of the above theorem, we have

$$\rho_A = \psi^\dagger\Gamma_A\psi = tr(\rho\Gamma_A) = \omega_A.$$

Therefore we can rewrite the above given identities as

$$\rho_I\rho_J = \frac{1}{D}\sum_{K,L}C_{KILJ}\rho_K\rho_L, \qquad \text{where} \quad \rho_A = \psi^\dagger\Gamma_A\psi.$$

Corollary 4.6. *Let $\mathcal{E} \equiv \otimes_{i=1}^n\mathcal{E}_i$ be a composite state space of complex D=2^n-dimension, and let ρ be an arbitrary $D \times D$ density operator. Then the following conditions are equivalent.*

(1) *ρ is in a pure state,*

(2) *$rank(\rho) = 1$,*

(3) *$tr(\rho^2) = 1$,*

(4) *For any ω_A defined by $\omega_A = tr(\rho\Gamma_A)$, the following identities are satisfied:*

$$\omega_I\omega_J = \frac{1}{D}\sum_{K,L}C_{KILJ}\omega_K\omega_L.$$

Proof. Obvious from Definition 2.2, Corollary 2.2, Theorem 4.4 and Theorem 4.5. □

4.3 Fibre bundle $S^{2D-1} \to \mathbb{CP}^{D-1}$, passage from n-qubit pure states to $D \times D$ pure density operators

First of all, note that, since $Mat(D, \mathbb{C})$ is a D^2-dimensional complex Hilbert space with the Clifford algebra inner product, it naturally becomes a D^2-dimensional Kähler manifold, which is a complex manifold equipped with a Kähler metric. Therefore $Mat(D, \mathbb{C})$ can also be regarded as a $2D^2$-dimensional Riemannian manifold, which is a real manifold endowed with a Riemannian metric. (For the details of Kähler manifolds and Riemannian manifolds, see for example [10] or [20].) In addition, the real vector space $H(D, \mathbb{C})$ of all $D \times D$ Hermitian matrices becomes a D^2-dimensional Riemannian manifold as a submanifold of $Mat(D, \mathbb{C})$.

We now return to the map

$$\begin{array}{rcccl} \widetilde{h}: & \mathcal{E} = \otimes_{i=1}^{n} \mathcal{E}_i & \longrightarrow & H(D, \mathbb{C}) & \subset \; Mat(D, \mathbb{C}) \\ & \psi & \longmapsto & \psi\psi^{\dagger} = \rho & \end{array},$$

where $N = 2n$, $D = 2^n$, ψ is an arbitrary vector in a composite Hilbert space $\mathcal{E}$, ρ is the corresponding Hermitian operator, $\rho_I = \psi^{\dagger}\Gamma_I\psi$ and $\Gamma_I \in \{\Gamma_A\}$.

However, this time let us concentrate only on pure states. Namely, we consider the restriction of the map $\widetilde{h}$ to the set of all state vectors, which are unit vectors. Obviously the domain becomes S^{2D-1}. (Remember that $\mathcal{E}$ can be regarded as a $2D$-dimensional real Hilbert space.) Then, by the map $\widetilde{h}|_{S^{2D-1}}$, every state vector is mapped to a *pure* density operator. In fact, from the normalisation condition $\psi^{\dagger}\psi = 1$, we have

$$tr(\rho) = tr(\psi\psi^{\dagger}) = \psi^{\dagger}\psi = 1.$$

Furthermore, for any D-dimensional complex vector v in $\mathcal{E}$,

$$v^{\dagger}\rho v = v^{\dagger}(\psi\psi^{\dagger})v = (\psi^{\dagger}v)^{\dagger}\psi^{\dagger}v = (\psi^{\dagger}v)^{*}\psi^{\dagger}v = |\psi^{\dagger}v|^2 \geq 0,$$

so that ρ is positive. Therefore ρ is exactly a density operator. In addition, by Corollary 2.2, ρ is pure since

$$tr(\rho^2) = tr(\psi\psi^{\dagger}\psi\psi^{\dagger}) = \psi^{\dagger}\psi\psi^{\dagger}\psi = (\psi^{\dagger}\psi)^2 = 1.$$

Conversely the definition of a pure density operator guarantees that every pure density operator ρ has a inverse image $\widetilde{h}^{-1}(\rho) = \psi$. This means that the image $\widetilde{h}(S^{2D-1})$ and the set of all pure density operators are exactly the same as a subset of $H(D,\mathbb{C})$. Therefore we put $\mathcal{Q}_D \equiv \widetilde{h}(S^{2D-1})$; then from now on, we regard $\mathcal{Q}_D$ as the set of all $D \times D$ pure density operators.

Clearly $\mathcal{Q}_D$ is neither an algebra nor a vector space. However, surprisingly and crucially, it turns out that the set $\mathcal{Q}_D$ is equivalent to the complex projective space $\mathbb{CP}^{D-1}$ as a $(2D-2)$-dimensional real manifold.

To see this more precisely, we first show that $\mathcal{Q}_D$ is equivalent to $\mathbb{CP}^{D-1}$ as sets, namely we construct a bijection between them.

Lemma 4.7. *There exists a bijection f such that*

$$\begin{array}{rccc} f: & \mathcal{Q}_D & \xrightarrow{\cong} & \mathbb{CP}^{D-1} \\ & \rho = \psi\psi^\dagger & \longmapsto & z \equiv [z_1 : z_2 : \cdots : z_D] \end{array}, \tag{4.18}$$

where $\psi = {}^t(z_1 \cdots z_D) \in S^{2D-1}$.

Proof. Firstly suppose that $\rho \in \mathcal{Q}_D$, that is, ρ is a $D \times D$ pure density operator. Then, by definition, there always exists a state vector $\psi = {}^t(z_1 \cdots z_D) \in S^{2D-1}$ such that

$$\rho = \psi\psi^\dagger = \begin{pmatrix} |z_1|^2 & z_1 z_2{}^* & \cdots & z_1 z_{D-1}{}^* & z_1 z_D{}^* \\ z_2 z_1{}^* & |z_2|^2 & \cdots & z_2 z_{D-1}{}^* & z_2 z_D{}^* \\ \vdots & \vdots & & \vdots & \vdots \\ z_{D-1} z_1{}^* & z_{D-1} z_2{}^* & \cdots & |z_{D-1}|^2 & z_2 z_D{}^* \\ z_D z_1{}^* & z_D z_2{}^* & \cdots & z_D z_{D-1}{}^* & |z_D|^2 \end{pmatrix}. \tag{4.19}$$

Now note that, since $|\psi|^2 = \sum_{i=1}^D |z_i|^2 = 1$, at least one of z_i is non-zero. For each non-zero z_i, the homogeneous coordinates (see Appendix A) of the i-th column are

$$\begin{aligned} & [z_1 z_i{}^* : \cdots : z_{i-1} z_i{}^* : |z_i|^2 : z_{i+1} z_i{}^* : \cdots : z_D z_i{}^*] \\ = \ & [z_1 : \cdots : z_{i-1} : z_i : z_{i+1} : \cdots : z_D], \end{aligned}$$

which means each set of homogeneous coordinates represents the same element $[z_1 : \cdots : z_n]$ in $\mathbb{CP}^{D-1}$. Therefore, for any $D \times D$ pure density operator ρ, there exists one and only one corresponding element $z \equiv [z_1 : \cdots : z_D]$ in $\mathbb{CP}^{D-1}$, and this means that f is well-defined by $f(\rho) \equiv z$.

Conversely, for any element $z = [z_1 : \cdots : z_D]$, in $\mathbb{CP}^{D-1}$, we can always find the corresponding density operator ρ by defining it by the equation (4.19). Note that we can choose a representative element $(z_1, \ldots, z_D)$ from S^{2D-1}, so that $\sum_{i=1}^D |z_i|^2 = 1$, which guarantees that $tr(\rho) = 1$. Furthermore this ρ does not depend on the choice of a representative element for z. In fact, for $\left[e^{i\chi}z_1 : \cdots : e^{i\chi}z_D\right]$, which is equal to $[z_1 : \cdots : z_D]$, we have the same corresponding density operator ρ since

$$\begin{pmatrix} |e^{i\chi}z_1|^2 & (e^{i\chi}z_1)(e^{i\chi}z_2)^* & \cdots & (e^{i\chi}z_1)(e^{i\chi}z_D)^* \\ (e^{i\chi}z_2)(e^{i\chi}z_1)^* & |e^{i\chi}z_2|^2 & \cdots & (e^{i\chi}z_2)(e^{i\chi}z_D)^* \\ \vdots & \vdots & & \vdots \\ (e^{i\chi}z_D)(e^{i\chi}z_1)^* & (e^{i\chi}z_D)(e^{i\chi}z_2)^* & \cdots & |e^{i\chi}z_D|^2 \end{pmatrix} = \rho.$$

Therefore the map f^{-1} is well-defined. Hence f is a bijection. □

Now we consider the C^∞-differential structures, which are structures as smooth (or C^∞-differentiable) manifolds, on $\mathcal{Q}_D$ and $\mathbb{CP}^{D-1}$. As we see in Appendix A, $\mathbb{CP}^{D-1}$ is a $(D-1)$-dimensional complex manifold, so that it can also be regarded as a $(2D-2)$-dimensional smooth real manifold. On the other hand, $\mathcal{Q}_D$ is also, in its own right, a smooth real manifold, as a submanifold of the D^2-dimensional smooth real manifold $H(D,\mathbb{C})$. To be more precise, since, for the n-qubit case, we have $(D-1)^2$ independent Fierz identities and the normalisation condition $\rho_0 = 1$, each of which defines a 1-codimensional hypersurface[6] in $H(D,\mathbb{C})$. Then $\mathcal{Q}_D$ becomes a smooth submanifold of $H(D,\mathbb{C})$, which is obtained as the intersection of all such hypersurfaces. Furthermore the number of independent components of $\mathcal{Q}_D$ is $D^2-(D-1)^2-1 = 2D-2$. Therefore $\mathcal{Q}_D$ becomes a $(2D-2)$-dimensional smooth real manifold.

Then the question is whether $\mathcal{Q}_D$ and $\mathbb{CP}^{D-1}$ are diffeomorphic. In other words, is the bijection f a diffeomorphism[7] between the two smooth manifolds?

Theorem 4.8. *Let f be the bijection defined in Lemma 4.7. Then f is a diffeomorphism between the two smooth manifolds $\mathcal{Q}_D$ and $\mathbb{CP}^{D-1}$.*

Proof. Recall, from Theorem A.1, that we can construct the D copies of coordinate systems $\{(U_j,\zeta_j)\}_{j=1,..,D}$ of the $(D-1)$-dimensional complex manifold $\mathbb{CP}^{D-1}$. Then, for $z \in U_j = \left\{z \in \mathbb{CP}^{D-1} \mid z_j \neq 0\right\}$, we have the composite map

$$f^{-1}\circ\zeta_j^{-1} : \begin{array}{ccccc} \mathbb{C}^{D-1} & \xrightarrow{\zeta_j^{-1}} & U_j & \xrightarrow{f^{-1}} & \mathcal{Q}_D \\ \zeta_j & \longmapsto & z & \longmapsto & \rho = \psi\psi^\dagger = (z_k z_l{}^*) \end{array}, \tag{4.20}$$

[6]The zero set of a single real polynomial in arbitrary dimension n is called a ***hypersurface*** in $\mathbb{R}^n$ (see [19] for more details).

[7]A ***diffeomorphism*** of a smooth (or C^∞-differentiable) manifold $\mathcal{M}$ onto another smooth manifold $\mathcal{N}$ is a bijection f such that both f and f^{-1} are smooth [9].

where $z = [z_1 : \cdots : z_D]$, $\zeta_j = \left(\zeta_j^1, \dots \zeta_j^{j-1}, \zeta_j^{j+1}, \dots \zeta_j^D\right)$ and $\zeta_j^k = z_k/z_j$. Obviously the map $f^{-1} \circ \zeta_j^{-1}$ is a bijection onto its image.

Now, for the (k, l)-entry $z_k z_l{}^*$ of ρ, we have

$$\begin{aligned} z_k z_l{}^* &= |z_j|^2 \frac{z_k}{z_j} \frac{z_l{}^*}{z_j{}^*} = \frac{|z_j|^2}{\sum_m |z_m|^2} \left(\frac{z_k}{z_j}\right) \left(\frac{z_l}{z_j}\right)^* \\ &= \left(\frac{\sum_m |z_m|^2}{|z_j|^2}\right)^{-1} \left(\frac{z_k}{z_j}\right) \left(\frac{z_l}{z_j}\right)^* \\ &= \left(\sum_m \left|\frac{z_m}{z_j}\right|^2\right)^{-1} \left(\frac{z_k}{z_j}\right) \left(\frac{z_l}{z_j}\right)^* \\ &= \frac{\zeta_j^k \zeta_j^{l*}}{\sum_m |\zeta_j^m|^2}, \end{aligned}$$

where m runs over the indices which give $z_m \neq 0$, so that $\sum_m |z_m|^2 = 1$ and $\zeta_j^m \neq 0$. This shows that the map $f^{-1} \circ \zeta_j^{-1}$ is a biholomorphism[8], and therefore a diffeomorphism, onto its image. Hence f is a diffeomorphism between $\mathcal{Q}_D$ and $\mathbb{CP}^{D-1}$. □

Then the next question should be whether $\mathcal{Q}_D$ is equivalent to $\mathbb{CP}^{D-1}$ as a Riemannian manifold, which is a real manifold with a Riemannian metric. (For more details, see for example [20].) In other words, whether the map f is an isometry[9] between $\mathcal{Q}_D$ and $\mathbb{CP}^{D-1}$. As we see in Appendix A, $\mathbb{CP}^{D-1}$ is a Kähler manifold endowed with the Fubini-Study metric, so that it can be also regarded as a Riemannian manifold. On the other hand, $\mathcal{Q}_D$ is also equipped with a Riemannian metric naturally induced from the Clifford algebra metric. Then, are the two metrics related by the map f? Unfortunately we are not ready to answer the question in a satisfactorily convincing manner except for the single qubit case, since we have not and will not provide sufficiently rigorous discussion on the Riemannian structure of the set $\mathcal{Q}_D$ of all $D \times D$ pure density operators in this thesis.

[8]A ***biholomorphism*** between two complex manifolds is a bijective holomorphic (or analytic) map whose inverse is also holomorphic [10].

[9]An ***isometry*** is a metric-preserving diffeomorphism between two Riemannian manifolds (for a more rigorous definition, see, for example, [9]).

Now we define the map h as $h \equiv f \circ \widetilde{h}|_{S^{2D-1}}$, namely

$$\begin{array}{ccccccc} h: & S^{2D-1} & \overset{\widetilde{h}|_{S^{2D-1}}}{\longrightarrow} & \widetilde{h}(S^{2D-1}) & \overset{f}{\longrightarrow} & \mathbb{CP}^{D-1} \\ & \psi = \begin{pmatrix} z_1 \\ \vdots \\ z_D \end{pmatrix} & \longmapsto & \rho = \psi\psi^\dagger & \longmapsto & z = [z_1 : \cdots : z_D] \end{array} . \tag{4.21}$$

This map h is no more than the projection for the fibre bundle $S^{2D-1} \longrightarrow \mathbb{CP}^{D-1}$ (see Appendix A). Note that, evidently, $(e^{i\chi}\psi)^\dagger(e^{i\chi}\psi) = \psi^\dagger\psi = \rho$ indicates that its fibre is S^1.

4.4 The two formulations of quantum mechanics and the map $h : S^{2D-1} \to \mathbb{CP}^{D-1}$

Let us recall the two formulations of quantum mechanics. In this section, we see that, for pure states, the two formulations are completely related by the map $h : S^{2D-1} \longrightarrow \mathbb{CP}^{D-1}$. Therefore, throughout this section, we assume that all quantum states are pure.

In Postulate 1 of the state vector formulation, a state vector, say $|\psi\rangle$, is employed to describe a physical system while, in Postulate 1' of the density operator formulation, a density operator ρ plays the equivalent role. Then $|\psi\rangle$ and ρ are clearly related to each other by the projection h since $\rho = |\psi\rangle\langle\psi|$.

In Postulate 2, the time evolution is described as

$$|\psi'\rangle = U|\psi\rangle, \tag{4.22}$$

with a unitary matrix U. Then, by the map h, we have pure density operators

$$\rho = |\psi\rangle\langle\psi| \quad \text{and} \quad \rho' = |\psi'\rangle\langle\psi'|.$$

However, by the equation (4.22),

$$\rho' = |\psi'\rangle\langle\psi'| = U|\psi\rangle\langle\psi|U^\dagger = U\rho U^\dagger.$$

This is precisely Postulate 2' of the density operator formulation.

In Postulate 3 in the state vector formulation, the probability for the measurement result m is given by

$$p(m) = \langle\psi|{M_m}^\dagger M_m|\psi\rangle.$$

Since $\rho = |\psi\rangle\langle\psi|$ for pure states,

$$\langle\psi|{M_m}^\dagger M_m|\psi\rangle = tr({M_m}^\dagger M_m|\psi\rangle\langle\psi|) = tr({M_m}^\dagger M_m\rho).$$

This agrees exactly with

$$p(m) = tr({M_m}^\dagger M_m\rho),$$

which is given in Postulate 3' in the density operator formulation. In addition, the state vector immediately after the measurement is

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|{M_m}^\dagger M_m|\psi\rangle}},$$

and it is mapped, by the projection h, to the density operator

$$\frac{M_m|\psi\rangle\langle\psi|{M_m}^\dagger}{\langle\psi|{M_m}^\dagger M_m|\psi\rangle} = \frac{M_m\rho{M_m}^\dagger}{tr({M_m}^\dagger M_m\rho)}.$$

Therefore Postulate 3 and Postulate 3' are related completely by the map h.

Lastly, let us consider Postulate 4 and Postulate 4'. Due to a basic property of tensor products,

$$(\otimes_{i=1}^{n}|\psi_i\rangle)\,(\otimes_{i=1}^{n}\langle\psi_i|) = \otimes_{i=1}^{n}|\psi_i\rangle\langle\psi_i| = \otimes_{i=1}^{n}\varrho_i.$$

This shows that, by the map h, the joint state vector $|\psi_1\rangle\otimes|\psi_2\rangle\otimes\cdots\otimes|\psi_n\rangle$ goes to the joint density operator $\varrho_1\otimes\varrho_2\otimes\cdots\otimes\varrho_n$. Hence the two Postulates are equivalent.

Remark. In Postulate 3', it can be seen that, by the equation (4.2), the probability $p(m)$ is nothing other than D times the inner product $\langle{M_m}^\dagger M_m, \rho\rangle_C$ of the matrices ${M_m}^\dagger M_m$ and ρ in terms of the Clifford algebra inner product. In particular, if ρ is in a pure state (*i.e.* $tr(\rho^2) = 1$), the size $\|\rho\|_C$ of ρ is:

$$\|\rho\|_C = \sqrt{\frac{1}{D}tr(\rho^2)} = \frac{1}{\sqrt{D}}, \tag{4.23}$$

and the size of the component of ρ in the $M_m^\dagger M_m$ direction is

$$\sqrt{\left\langle M_m^\dagger M_m, \rho\right\rangle_C} = \sqrt{\frac{1}{D}tr(M_m^\dagger M_m\rho)} = \sqrt{\frac{1}{D}p(m)}. \tag{4.24}$$

Furthermore recall that, for the pure state case, we have $\rho_I = \omega_I$, where $\rho_I = \langle\psi|\Gamma_I|\psi\rangle$, $\omega_I = tr(\rho\Gamma_I)$ and Γ_I is a basis element of $H(D,\mathbb{C})$. Therefore, from the equations (4.7) and (4.23),

$$\sum_I {\rho_I}^2 = \sum_I {\omega_I}^2 = D. \tag{4.25}$$

5 Single qubit states

This Chapter is devoted to the single qubit case, which includes not only the pure state case but also the mixed state case, as the most simple example of our Clifford algebra description of quantum states. In the first section, the Clifford algebra $Cl_2(\mathbb{C})$ and its matrix representation $Mat(2, \mathbb{C})$ are discussed in a explicit way. Then, in the second section, we focus on the pure state case to derive the first Hopf bundle $S^3 \to S^2$. In the next section, we turn our eyes to single qubit mixed states, and introduce a measure for 'mixedness' of a single qubit state. In the closing section, we consider the Riemannian structure of the space $\mathcal{Q}_2$ of all 2×2 pure density operators, and show that $\mathcal{Q}_2$ is naturally identified with the complex projective space $\mathbb{CP}^1$ as a Riemannian manifold.

5.1 The space of single qubit states and its coordinates

In the case of single qubit states, our complex Clifford algebra is $Cl_2(\mathbb{C})$ and the basis for its matrix representation $\tau(Cl_2(\mathbb{C})) \cong Mat(2, \mathbb{C})$ is $\{\mathbb{I}, \Gamma_1, \Gamma_2, \widetilde{\Gamma}\}$ as seen in Example 3.3. Since we consider both pure state and mixed state cases, a density operator ρ does not always have a state vector $\psi \in \mathcal{E}$ such that $\psi\psi^\dagger = \rho$. Therefore we can not define the quadratic forms $\{\rho_A\}$ at all times. Thus we rather employ $\{\omega_A\}$, which was defined by $\omega_A = tr(\rho\Gamma_A)$ in Theorem 4.2.

Remark. Unlike Theorem 4.2, ρ is assumed to be a density operator throughout this section and the next section, so that it is Hermitian. Therefore

$$\begin{aligned} \omega_A{}^* &= (tr(\rho\Gamma_A))^* = tr\left((\rho\Gamma_A)^\dagger\right) = tr(\Gamma_A{}^\dagger\rho^\dagger) \\ &= tr(\Gamma_A\,\rho) = tr(\rho\Gamma_A) = \omega_A. \end{aligned} \tag{5.1}$$

Hence every ω_A is real.

For a generic 2×2 density operator ρ, from Theorem 4.2 and the condition $tr(\rho) = 1$,

$$\rho = \frac{1}{2}\left(I + \omega_1\Gamma_1 + \omega_2\Gamma_2 + \widetilde{\omega}\widetilde{\Gamma}\right),$$

where $\omega_A = tr(\rho\Gamma_A)$. Then we have the following theorem.

Theorem 5.1. *Let ρ be an arbitrary 2×2 density operator, and $\omega_A = tr(\rho\Gamma_A)$. Then*

$$\omega_1{}^2 + \omega_2{}^2 + \widetilde{\omega}^2 \leq 1, \tag{5.2}$$

with equality if and only if ρ is in a pure state. Alternatively, ${\omega_1}^2+{\omega_2}^2+\widetilde{\omega}^2 < 1$ if and only if ρ is in a mixed state. Furthermore, if ρ is in a pure state, then $\omega_A = \rho_A$, so that

$$ {\rho_1}^2 + {\rho_2}^2 + \widetilde{\rho}^2 = 1. \tag{5.3} $$

Proof. Firstly suppose that ρ is an arbitrary 2×2 density operator. Since we have already proved Corollary 2.2, it is sufficient to show that the conditions $tr(\rho^2) \leq 1$ and ${\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2 \leq 1$ are equivalent. Now $\rho = \frac{1}{2}\left(I + \omega_1\Gamma_1 + \omega_2\Gamma_2 + \widetilde{\omega}\widetilde{\Gamma}\right)$ and Theorem 4.1 imply that

$$ \begin{aligned} tr(\rho^2) &= tr\left[\frac{1}{4}\left(I^2 + {\omega_1}^2{\Gamma_1}^2 + {\omega_2}^2{\Gamma_2}^2 + \widetilde{\omega}^2\widetilde{\Gamma}^2\right)\right] \\ &= \frac{1}{4}\left(1 + {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2\right) trI \\ &= \frac{1}{2}\left(1 + {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2\right). \end{aligned} $$

Then $tr(\rho^2) \leq 1$ leads to

$$ \begin{aligned} \frac{1}{2}\left(1 + {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2\right) &\leq 1 \\ {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2 &\leq 1. \end{aligned} $$

Conversely $tr(\rho^2) \leq 1$ can be derived from ${\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2 \leq 1$ in a similar manner. Therefore these two conditions are equivalent.

Now let us suppose that ρ is in a pure state. In this case, for any pure density operator ρ, there exist a state vector $\psi \in \mathcal{E}$ such that $\rho = \psi\psi^\dagger$. Hence

$$ \omega_A = tr(\rho\Gamma_A) = tr(\psi\psi^\dagger\Gamma_A) = tr(\psi^\dagger\Gamma_A\psi) = \rho_A. $$

Consequently

$$ {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2 = {\rho_1}^2 + {\rho_2}^2 + \widetilde{\rho}^2 = 1. $$

□

Remark. Since every ω_A is real for the single qubit case as seen above,

$$ {\omega_1}^2 + {\omega_2}^2 + \widetilde{\omega}^2 \geq 0. \tag{5.4} $$

Now let us develop this discussion in a more explicit way. As we have already seen in Example 3.3, the basis for the matrix representation $\tau(Cl_2(\mathbb{C})) \cong Mat(2, \mathbb{C})$ may be $\{\mathbb{I}, \Gamma_1, \Gamma_2, \widetilde{\Gamma}\}$, where $\Gamma_1 = \sigma_1$, $\Gamma_2 = \sigma_2$ and $\widetilde{\Gamma} = -\sigma_3$.

Then it is straightforward to see that the $\{\omega_A\}$ become:

$$\begin{aligned}
\omega_0 &= tr(\rho) = |\alpha|^2 + |\beta|^2 = 1, \\
\omega_1 &= tr(\rho\Gamma_1) = tr(\rho\sigma_1) = \alpha^*\beta + \beta^*\alpha = 2Re(\alpha^*\beta), \\
\omega_2 &= tr(\rho\Gamma_2) = tr(\rho\sigma_2) = -i(\alpha^*\beta - \beta^*\alpha) = 2Im(\alpha^*\beta), \\
\widetilde{\omega} &= tr(\rho\Gamma_3) = tr(\rho(-\sigma_3)) = |\beta|^2 - |\alpha|^2.
\end{aligned} \tag{5.5}$$

Furthermore the density matrix ρ becomes

$$\begin{aligned}
\rho &= \frac{1}{2}\left(I + \omega_1\Gamma_1 + \omega_2\Gamma_2 + \widetilde{\omega}\widetilde{\Gamma}\right) \\
&= \frac{1}{2}\begin{pmatrix} 1+\widetilde{\omega} & \omega_1 - i\omega_2 \\ \omega_1 + i\omega_2 & 1-\widetilde{\omega} \end{pmatrix} \\
&= U\begin{pmatrix} \frac{1+r}{2} & 0 \\ 0 & \frac{1-r}{2} \end{pmatrix} U^\dagger,
\end{aligned} \tag{5.6}$$

where $r = \sqrt{\omega_1{}^2 + \omega_2{}^2 + \widetilde{\omega}^2}$ and

$$U = \frac{1}{\sqrt{2r(r+\widetilde{\omega})}}\begin{pmatrix} r+\widetilde{\omega} & -\omega_1 + i\omega_2 \\ \omega_1 + i\omega_2 & r+\widetilde{\omega} \end{pmatrix}.$$

Remark. From the last line of the equation (5.6), it is clear that the following four conditions are equivalent:

(i) ρ is in a pure state,

(ii) $\omega_1{}^2 + \omega_2{}^2 + \widetilde{\omega}^2 = 1$,

(iii) $rank(\rho) = 1$,

(iv) $det(\rho) = 0$.

5.2 Single qubit pure states and the fibre bundle structure

Now we concentrate on the pure state case. In this case, our quadratic forms $\{\rho_A\}$ can be safely defined, and, as we have seen, $\rho_A = \omega_A$. Therefore ρ is written as

$$\rho = \frac{1}{2}\left(\rho_0 I + \rho_1\Gamma_1 + \rho_2\Gamma_2 + \widetilde{\rho}\widetilde{\Gamma}\right),$$

where $\rho = \psi\psi^\dagger$ for some $\psi \in \mathcal{E}$. Furthermore, from Theorem 4.4, it turns out that we have only one Fierz identity:

$$\rho_0{}^2 = \rho_1{}^2 + \rho_2{}^2 + \widetilde{\rho}^2, \tag{5.7}$$

and together with the normalisation condition $\rho_0 = 1$ (which is merely equivalent to $|\psi| = 1$); this equation becomes

$$\rho_1{}^2 + \rho_2{}^2 + \widetilde{\rho}^2 = 1,$$

which is nothing but the necessary and sufficient condition for the fact that ρ is pure.

Geometrically the Fierz identity $\rho_0{}^2 = \rho_1{}^2 + \rho_2{}^2 + \widetilde{\rho}^2$ represents a 3-dimensional hypercone, and the normalisation condition $\rho_0 = 1$ represents a 3-dimensional hyperplane, both in the 4-dimensional real vector space $H(2, \mathbb{C})$. Then the intersection of these hypersurfaces is the Bloch sphere S^2 (see page 10 and Appendix B), which is represented by simultaneous equations $\rho_0{}^2 = \rho_1{}^2 + \rho_2{}^2 + \widetilde{\rho}^2$ and $\rho_0 = 1$. Furthermore the Bloch sphere is identified with the space $\mathcal{Q}_2$ of single qubit pure states, which is diffeomorphic to $\mathbb{CP}^1$.

Then, from the equation (5.5) and $\rho_A = \omega_A$, the quadratic forms $\{\rho_A\}$ become:

$$\begin{aligned} &\rho_0 = |\alpha|^2 + |\beta|^2 = 1, \\ &\rho_1 = \alpha^*\beta + \beta^*\alpha = 2Re(\alpha^*\beta), \\ &\rho_2 = -i(\alpha^*\beta - \beta^*\alpha) = 2Im(\alpha^*\beta), \\ &\widetilde{\rho} = |\beta|^2 - |\alpha|^2. \end{aligned} \tag{5.8}$$

Note that the above coordinates are precisely the same as the coordinates for the Bloch sphere given in Theorem B.1. In fact, the map

$$h: \begin{array}{ccccc} S^3 & \xrightarrow{h} & \mathbb{CP}^1 & \xrightarrow{\cong} & S^2 \\ \psi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} & \longmapsto & [\alpha : \beta] & \longmapsto & (\rho_1, \rho_2, \widetilde{\rho}) \end{array} \tag{5.9}$$

is nothing other than the projection (B.4) for the first Hopf bundle. In addition, the map $\mathbb{CP}^1 \longrightarrow S^2$ is identical with the map π in Theorem B.1.

5.3 Single qubit mixed states and the 'mixedness' $\mathcal{M}(\rho)$

What about if ρ is in a mixed state? Theorem 5.1 indicates that, for mixed states, each density operator can be represented as a point in the open Bloch 'ball' B^3, which is the interior of the Bloch sphere and represented by

$$\omega_1{}^2 + \omega_2{}^2 + \widetilde{\omega}^2 < 1 \quad \text{and} \quad \omega_0 = 1. \tag{5.10}$$

Furthermore, interestingly, a function

$$\mathcal{M}(\rho) \equiv 2\sqrt{det(\rho)} = \sqrt{1-({\omega_1}^2+{\omega_2}^2+\widetilde{\omega}^2)} = \sqrt{1-r^2} \tag{5.11}$$

can be employed as a measurement tool for 'mixedness' of a density operator just like the well-known von Neumann entropy. To be more precise, the von Neumann entropy $\mathcal{S}(\rho)$ is defined as

$$\mathcal{S}(\rho) \equiv -tr\,(\rho \log_2 \rho) = -\sum_x \lambda_x \log_2 \lambda_x, \tag{5.12}$$

where λ_x are the eigenvalues of ρ, and $0 \log_2 0 \equiv 0$. Note that Theorem 5.1 and the equation (5.4) indicate

$$0 \leq \mathcal{M}(\rho) \leq 1. \tag{5.13}$$

In the case of single qubit states, we have $\mathcal{S}(\rho) = 0$ for pure states and $0 < \mathcal{S}(\rho) \leq 1$ for mixed states. Our $\mathcal{M}(\rho)$ has exactly the same property. That is, $\mathcal{M}(\rho) = 0$ for pure states and $0 < \mathcal{M}(\rho) \leq 1$ for mixed states. Moreover it turns out that, as $\mathcal{S}(\rho)$ increases, $\mathcal{M}(\rho)$ also increases monotonically, and $\mathcal{M}(\rho) = 1$ when ρ is *maximally mixed* (i.e. $\mathcal{S}(\rho) = 1$). This means that the maximally mixed state is located in the centre of the Bloch 'ball' ($r = 0$), and as the states are situated more distant from the centre, they become less mixed. Then, finally, on the boundary: ${\rho_1}^2 + {\rho_2}^2 + \widetilde{\rho}^2 = 1$ and $\rho_0 = 1$ ($r = 1$), the states become pure.

Now we provide a rigorous proof for the fact that, as $\mathcal{S}(\rho)$ increases, $\mathcal{M}(\rho)$ also increases monotonically. (However it is just elementary calculus). To prove this, it is sufficient to show that, regarding $\mathcal{S}(\rho)$ as a function of $\mathcal{M}(\rho)$,

$$\frac{d\mathcal{S}}{d\mathcal{M}} > 0, \qquad \text{if } \ 0 < \mathcal{M}(\rho) < 1 \ \text{ (or equivalently } 0 < r < 1).$$

In this case, from the equation (5.6) and(5.12),

$$\mathcal{S}(\rho) = -\frac{1+r}{2}\log_2\frac{1+r}{2} - \frac{1-r}{2}\log_2\frac{1-r}{2}.$$

Thus

$$\frac{d\mathcal{S}}{dr} = -\frac{1}{\ln 2} - \frac{1}{2}\log_2\frac{1+r}{1-r}.$$

Meanwhile, from $\mathcal{M}(\rho) = \sqrt{1-r^2}$, we have

$$\frac{d\mathcal{M}}{dr} = -\frac{r}{\sqrt{1-r^2}}.$$

Hence

$$\begin{aligned}
\frac{d\mathcal{S}}{d\mathcal{M}} &= \frac{d\mathcal{S}}{dr}\cdot\frac{dr}{d\mathcal{M}} = \left(-\frac{1}{\ln 2} - \frac{1}{2}\log_2\frac{1+r}{1-r}\right)\cdot\left(-\frac{\sqrt{1-r^2}}{r}\right) \\
&= \frac{\sqrt{1-r^2}}{r}\left(\frac{1}{\ln 2} + \frac{1}{2}\log_2\frac{1+r}{1-r}\right).
\end{aligned}$$

Here $0 < r < 1$ leads to

$$\frac{\sqrt{1-r^2}}{r} > 0, \quad \frac{1+r}{1-r} > 1, \quad \text{and then,} \quad \log_2\frac{1+r}{1-r} > 0.$$

Hence $d\mathcal{S}/d\mathcal{M} > 0$, so that the claim is proved.

5.4 Clifford algebra metric and Fubini-Study metric

Throughout this section, we assume that, for an operator ρ, there exist a vector $\psi \in \mathcal{E}$ such that $\rho = \psi\psi^\dagger$.

Let us now recall that $H(2,\mathbb{C})$ is a 4-dimensional vector space over $\mathbb{R}$ with the Clifford algebra inner product, so that it can be naturally regarded as a 4-dimensional Riemannian manifold with the coordinate functions $(\rho_0, \rho_1, \rho_2, \widetilde{\rho})$. Then its cotangent space at the origin, whose coordinates are $(d\rho_0, d\rho_1, d\rho_2, d\widetilde{\rho})$, is naturally identified with $H(2,\mathbb{C})$ itself together with its inner product, namely the Clifford algebra metric. Therefore the distance ds between two neighbouring points in $H(2,\mathbb{C})$ is obtained from

$$ds^2 = \sum_{I,J} G_{IJ}d\rho_I d\rho_J = d\rho_0{}^2 + d\rho_1{}^2 + d\rho_2{}^2 + d\widetilde{\rho}^2, \tag{5.14}$$

where (G_{IJ}) becomes the 4×4 identity matrix.

Since the Fierz identity $\rho_0{}^2 = \rho_1{}^2 + \rho_2{}^2 + \widetilde{\rho}^2$ represents a 3-dimensional hypercone, the above metric can be transformed by the following spherical polar coordinates:

$$\rho_1 = \rho_0\cos\theta, \qquad \rho_2 = \rho_0\sin\theta\cos\phi, \qquad \widetilde{\rho} = \rho_0\sin\theta\sin\phi.$$

Then we have

$$\begin{aligned}
d\rho_1 &= \cos\theta d\rho_0 - \rho_0\sin\theta d\theta, \\
d\rho_2 &= \sin\theta\cos\phi d\rho_0 + \rho_0\cos\theta\cos\phi d\theta - \rho_0\sin\theta\sin\phi d\phi, \\
d\widetilde{\rho} &= \sin\theta\sin\phi d\rho_0 + \rho_0\cos\theta\sin\phi d\theta + \rho_0\sin\theta\cos\phi d\phi.
\end{aligned}$$

Substituting these equations into (5.14), we have

$$ds^2 = 2d{\rho_0}^2 + {\rho_0}^2 \left(d\theta^2 + \sin^2\theta d\phi^2\right).$$

Finally, we take only pure density operators into account, and that leads to the normalisation condition $\rho_0 = 1$ and therefore $d\rho_0 = 0$. Then we have

$$ds^2 = d\theta^2 + \sin^2\theta d\phi^2. \tag{5.15}$$

This is the metric on the space $\mathcal{Q}_2$ of all 2×2 pure density operators naturally induced by the Clifford algebra metric. However this is nothing but the Fubini-Study metric in the complex projective space $\mathbb{CP}^1$ or, in other words, the standard round metric on the Riemann sphere (see Appendix A). This implies that $\mathcal{Q}_2$ can be identified with $\mathbb{CP}^1$ as a Riemannian manifold.

6 Two-qubit pure states

In this chapter, we take a close look at the two-qubit state case. However, unlike the single qubit state case, we consider only the case of pure states. In the first section of this chapter, we provide an explicit description of the space $\mathcal{Q}_4$ of 4×4 pure density operators in relation to the Fierz identities. In the next section, we develop the picture of $\mathcal{Q}_4$ by introducing the reduced density operators for the subsystems. In the last section, we provide a geometrical explanation for the "EPR paradox" in terms of our Clifford algebra description for the two-qubit pure states.

6.1 Two-qubit pure states and the fibre bundle structure

In the two-qubit case, the Clifford algebra in our discussion is $Cl_4(\mathbb{C})$ and its basis

$$\{\gamma_A\} = \{\mathbb{I}, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \widetilde{\gamma}_{12}, \widetilde{\gamma}_{13}, \widetilde{\gamma}_{14}, \widetilde{\gamma}_{23}, \widetilde{\gamma}_{24}, \widetilde{\gamma}_{34}, \widetilde{\gamma}_1, \widetilde{\gamma}_2, \widetilde{\gamma}_3, \widetilde{\gamma}_4, \widetilde{\gamma}\},$$

is obtained in an analogous way to Example 3.2 for $Cl_4(\mathbb{R})$. Then the representing matrix for each basis element may be

$$\mathbb{I} \simeq I \equiv I \otimes I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{6.1}$$

$$\gamma_1 \simeq \Gamma_1 \equiv \sigma_3 \otimes I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{6.2}$$

$$\gamma_2 \simeq \Gamma_2 \equiv \sigma_2 \otimes \sigma_1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \tag{6.3}$$

$$\gamma_3 \simeq \Gamma_3 \equiv \sigma_2 \otimes \sigma_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{6.4}$$

$$\gamma_4 \simeq \Gamma_4 \equiv \sigma_2 \otimes \sigma_3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \tag{6.5}$$

$$\widetilde{\gamma}_{12} \simeq \widetilde{\Gamma}_{12} \equiv i\Gamma_3\Gamma_4 = -I\otimes\sigma_1 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \tag{6.6}$$

$$\widetilde{\gamma}_{13} \simeq \widetilde{\Gamma}_{13} \equiv -i\Gamma_2\Gamma_4 = I\otimes\sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \tag{6.7}$$

$$\widetilde{\gamma}_{14} \simeq \widetilde{\Gamma}_{14} \equiv i\Gamma_2\Gamma_3 = -I\otimes\sigma_3 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{6.8}$$

$$\widetilde{\gamma}_{23} \simeq \widetilde{\Gamma}_{23} \equiv i\Gamma_1\Gamma_4 = \sigma_1\otimes\sigma_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \tag{6.9}$$

$$\widetilde{\gamma}_{24} \simeq \widetilde{\Gamma}_{24} \equiv -i\Gamma_1\Gamma_3 = -\sigma_1\otimes\sigma_2 = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \tag{6.10}$$

$$\widetilde{\gamma}_{34} \simeq \widetilde{\Gamma}_{34} \equiv i\Gamma_1\Gamma_2 = \sigma_1\otimes\sigma_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{6.11}$$

$$\widetilde{\gamma}_{1} \simeq \widetilde{\Gamma}_{1} \equiv -i\Gamma_2\Gamma_3\Gamma_4 = \sigma_2\otimes I = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \tag{6.12}$$

$$\widetilde{\gamma}_{2} \simeq \widetilde{\Gamma}_{2} \equiv i\Gamma_1\Gamma_3\Gamma_4 = -\sigma_3\otimes\sigma_1 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{6.13}$$

$$\widetilde{\gamma}_{3} \simeq \widetilde{\Gamma}_{3} \equiv -i\Gamma_1\Gamma_2\Gamma_4 = -\sigma_3\otimes\sigma_2 = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \tag{6.14}$$

$$\widetilde{\gamma}_{4} \simeq \widetilde{\Gamma}_{4} \equiv i\Gamma_1\Gamma_2\Gamma_3 = -\sigma_3\otimes\sigma_3 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{6.15}$$

$$\widetilde{\gamma} \simeq \widetilde{\Gamma} \equiv -\Gamma_1\Gamma_2\Gamma_3\Gamma_4 = -\sigma_1 \otimes I = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \quad (6.16)$$

Furthermore, by the definition (3.9), namely $\rho_A \equiv \psi^\dagger \Gamma_A \psi$, where $\psi = {}^t(\alpha, \beta, \gamma, \delta)$, we have the following 16 quadratic forms $\{\rho_A\}$:

$$\begin{aligned}
\rho_0 &= \psi^\dagger\psi = |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1, && (6.17)\\
\rho_1 &= \psi^\dagger(\sigma_3 \otimes I)\psi = |\alpha|^2 + |\beta|^2 - |\gamma|^2 - |\delta|^2, && (6.18)\\
\rho_2 &= \psi^\dagger(\sigma_2 \otimes \sigma_1)\psi = 2Im(\alpha^*\delta + \beta^*\gamma), && (6.19)\\
\rho_3 &= \psi^\dagger(\sigma_2 \otimes \sigma_2)\psi = -2Re(\alpha^*\delta - \beta^*\gamma), && (6.20)\\
\rho_4 &= \psi^\dagger(\sigma_2 \otimes \sigma_3)\psi = 2Im(\alpha^*\gamma - \beta^*\delta), && (6.21)\\
\widetilde{\rho}_{12} &= \psi^\dagger(-I \otimes \sigma_1)\psi = -2Re(\alpha^*\beta + \gamma^*\delta), && (6.22)\\
\widetilde{\rho}_{13} &= \psi^\dagger(I \otimes \sigma_2)\psi = 2Im(\alpha^*\beta + \gamma^*\delta), && (6.23)\\
\widetilde{\rho}_{14} &= \psi^\dagger(-I \otimes \sigma_3)\psi = -|\alpha|^2 + |\beta|^2 - |\gamma|^2 + |\delta|^2, && (6.24)\\
\widetilde{\rho}_{23} &= \psi^\dagger(\sigma_1 \otimes \sigma_3)\psi = 2Re(\alpha^*\gamma - \beta^*\delta), && (6.25)\\
\widetilde{\rho}_{24} &= \psi^\dagger(-\sigma_1 \otimes \sigma_2)\psi = 2Im(\alpha^*\delta - \beta^*\gamma), && (6.26)\\
\widetilde{\rho}_{34} &= \psi^\dagger(\sigma_1 \otimes \sigma_1)\psi = 2Re(\alpha^*\delta + \beta^*\gamma), && (6.27)\\
\widetilde{\rho}_1 &= \psi^\dagger(\sigma_2 \otimes I)\psi = 2Im(\alpha^*\gamma + \beta^*\delta), && (6.28)\\
\widetilde{\rho}_2 &= \psi^\dagger(-\sigma_3 \otimes \sigma_1)\psi = -2Re(\alpha^*\beta - \gamma^*\delta), && (6.29)\\
\widetilde{\rho}_3 &= \psi^\dagger(-\sigma_3 \otimes \sigma_2)\psi = -2Im(\alpha^*\beta - \gamma^*\delta), && (6.30)\\
\widetilde{\rho}_4 &= \psi^\dagger(-\sigma_3 \otimes \sigma_3)\psi = -|\alpha|^2 + |\beta|^2 + |\gamma|^2 - |\delta|^2, && (6.31)\\
\widetilde{\rho} &= \psi^\dagger(-\sigma_1 \otimes I)\psi = -2Re(\alpha^*\gamma + \beta^*\delta). && (6.32)
\end{aligned}$$

In the two-qubit pure state case, we expect to have 9 independent Fierz identities, since $D = 2^n = 2^2 = 4$ and $(D-1)^2 = (4-1)^2 = 9$ (see Section 4.2). To find these 9 Fierz identities, we use the condition $rank(\rho) = 1$, which is a necessary and sufficient condition for the existence of the Fierz identities shown in Corollary 4.6.

Lemma 6.1. *Let X be a 4×4 non-zero Hermitian matrix such that*

$$X = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{12}^* & a_{22} & a_{23} & a_{24} \\ a_{13}^* & a_{23}^* & a_{33} & a_{34} \\ a_{14}^* & a_{24}^* & a_{34}^* & a_{44} \end{pmatrix} \quad \textit{and} \quad a_{11} \neq 0.$$

Then, $rank(X) = 1$ if and only if the following 6 equations hold.

(i) $a_{11}a_{22} = |a_{12}|^2$

(ii) $a_{11}a_{33} = |a_{13}|^2$

(iii) $a_{11}a_{44} = |a_{14}|^2$

(iv) $a_{11}a_{23} = a_{13}a_{12}^*$

(v) $a_{11}a_{24} = a_{14}a_{12}^*$

(vi) $a_{11}a_{34} = a_{14}a_{13}^*$.

Proof. First of all, note that, since X is Hermitian, all of its diagonal entries are real. Namely, $a_{11}^* = a_{11}$, $a_{22}^* = a_{22}$, $a_{33}^* = a_{33}$ and $a_{44}^* = a_{44}$. Then it is easily seen that, by a finite number of rank-preserving operations on X, X can be changed into the Hermitian matrix

$$X' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & a_{11}a_{22} - |a_{12}|^2 & a_{11}a_{23} - a_{13}a_{12}^* & a_{11}a_{24} - a_{14}a_{12}^* \\ 0 & a_{11}a_{23}^* - a_{12}a_{13}^* & a_{11}a_{33} - |a_{13}|^2 & a_{11}a_{34} - a_{14}a_{13}^* \\ 0 & a_{11}a_{24}^* - a_{12}a_{14}^* & a_{11}a_{34}^* - a_{13}a_{14}^* & a_{11}a_{44} - |a_{14}|^2 \end{pmatrix}. \quad (6.33)$$

Now, if $rank(X) = rank(X') = 1$, then, evidently, the above 6 equations need to be satisfied. Conversely, if these 6 equations hold, then clearly $rank(X') = rank(X) = 1$. $\square$

Now we modify the above collection of 6 equations slightly in order to make our later calculation easier. It turns out that we can choose the following 6 equations instead of the above ones:

(i') $a_{11}a_{22} = |a_{12}|^2$

(ii') $a_{22}a_{33} = |a_{23}|^2$

(iii') $a_{33}a_{44} = |a_{34}|^2$

(iv') $a_{12}a_{34} = a_{14}a_{23}^*$

(v') $a_{13}a_{24} = a_{14}a_{23}$

(vi') $a_{12}^*a_{23}^* = a_{22}a_{13}^*$.

Here we show how we can obtain the identity (ii') as an example. The rest of the identities can be easily obtained in a similar manner.

From (i) and (ii),

$$a_{22} = \frac{|a_{12}|^2}{a_{11}} \quad \text{and} \quad a_{33} = \frac{|a_{13}|^2}{a_{11}}.$$

Then, since X is Hermitian and, therefore, a_{11} is real,

$$a_{22}a_{33} = \frac{|a_{12}|^2|a_{13}|^2}{|a_{11}|^2} = \frac{(a_{12}a_{13}{}^*)(a_{12}{}^*a_{13})}{|a_{11}|^2}.$$

Consequently, from (iv),

$$a_{22}a_{33} = \frac{(a_{11}^*a_{23}{}^*)(a_{11}a_{23})}{|a_{11}|^2} = \frac{|a_{11}|^2|a_{23}|^2}{|a_{11}|^2} = |a_{23}|^2.$$

Conversely the identities (i) to (vi) can be easily recovered from the identities (i') to (vi').

Now we rewrite the above equations (i') to (vi') for the two-qubit pure density operator

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* & \alpha\gamma^* & \alpha\delta^* \\ \alpha^*\beta & |\beta|^2 & \beta\gamma^* & \beta\delta^* \\ \alpha^*\gamma & \beta^*\gamma & |\gamma|^2 & \gamma\delta^* \\ \alpha^*\delta & \beta^*\delta & \gamma^*\delta & |\delta|^2 \end{pmatrix},$$

where $|\psi\rangle = {}^t(\alpha, \beta, \gamma, \delta)$. Then we have the following 6 equations:

(I) $\left(|\alpha|^2\right)\left(|\beta|^2\right) = (\alpha^*\beta)(\alpha\beta^*)$

(II) $\left(|\beta|^2\right)\left(|\gamma|^2\right) = (\beta^*\gamma)(\beta\gamma^*)$

(III) $\left(|\gamma|^2\right)\left(|\delta|^2\right) = (\gamma^*\delta)(\gamma\delta^*)$

(IV) $(\alpha^*\beta)(\gamma^*\delta) = (\alpha^*\delta)(\beta\gamma^*)$

(V) $(\alpha^*\gamma)(\beta^*\delta) = (\alpha^*\delta)(\beta^*\gamma)$

(VI) $(\alpha^*\beta)(\beta^*\gamma) = \left(|\beta|^2\right)(\alpha^*\gamma)$.

The above 6 equations are rewritten into the following 9 Fierz identities:

(F1) $\rho_0{}^2 = \rho_1{}^2 + \rho_2{}^2 + \rho_3{}^2 + \rho_4{}^2 + \widetilde{\rho}^2$

(F2) $\rho_0{}^2 = \widetilde{\rho}_1{}^2 + \widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}^2$

(F3) $\rho_0{}^2 = \rho_2{}^2 + \widetilde{\rho}_2{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 + \widetilde{\rho}_{34}{}^2$

(F4) $\rho_0\rho_1 + \widetilde{\rho}_{13}\widetilde{\rho}_3 = \widetilde{\rho}_{12}\widetilde{\rho}_2 + \widetilde{\rho}_{14}\widetilde{\rho}_4$

(F5) $\rho_0\widetilde{\rho}_4 = \rho_1\widetilde{\rho}_{14} + \rho_2\widetilde{\rho}_{24} + \rho_3\widetilde{\rho}_{34}$

(F6) $\rho_2\rho_3 = \widetilde{\rho}_{12}\widetilde{\rho}_3 + \widetilde{\rho}_{13}\widetilde{\rho}_2 + \widetilde{\rho}_{24}\widetilde{\rho}_{34}$

(F7) $\rho_3\widetilde{\rho}_{24} = \rho_2\widetilde{\rho}_{34} + \rho_4\widetilde{\rho}_{23} + \widetilde{\rho}_1\widetilde{\rho}$

(F8) $\rho_0\widetilde{\rho} + \rho_1\widetilde{\rho} + \widetilde{\rho}_{14}\widetilde{\rho} + \widetilde{\rho}_4\widetilde{\rho} + \rho_2\widetilde{\rho}_3 + \widetilde{\rho}_{24}\widetilde{\rho}_3 = \rho_0\widetilde{\rho}_{23} + \rho_1\widetilde{\rho}_{23}$
$+ \widetilde{\rho}_{14}\widetilde{\rho}_{23} + \widetilde{\rho}_4\widetilde{\rho}_{23} + \rho_2\widetilde{\rho}_{13} + \rho_3\widetilde{\rho}_{12} + \rho_3\widetilde{\rho}_2 + \widetilde{\rho}_{34}\widetilde{\rho}_2 + \widetilde{\rho}_{12}\widetilde{\rho}_{34} + \widetilde{\rho}_{13}\widetilde{\rho}_{24}$

(F9) $\rho_3\widetilde{\rho}_{13} + \widetilde{\rho}_{13}\widetilde{\rho}_{34} = \rho_0\rho_4 + \rho_0\widetilde{\rho}_1 + \rho_1\rho_4 + \rho_1\widetilde{\rho}_1 + \rho_4\widetilde{\rho}_{14} + \rho_4\widetilde{\rho}_4$
$+ \widetilde{\rho}_{14}\widetilde{\rho}_1 + \widetilde{\rho}_1\widetilde{\rho}_4 + \rho_2\widetilde{\rho}_{12} + \rho_2\widetilde{\rho}_2 + \rho_3\widetilde{\rho}_{34} + \rho_3\widetilde{\rho}_3 + \widetilde{\rho}_{12}\widetilde{\rho}_{24} + \widetilde{\rho}_{24}\widetilde{\rho}_2.$

The details of the calculation to derive the above 9 Fierz identities are shown in Appendix C.

Again, in this case, each Fierz identity, together with the normalisation condition $\rho_0 = 1$, define a hypersurface in the smooth manifold $H(4, \mathbb{C})$, and the intersection of all the hypersurfaces is the space $\mathcal{Q}_4$ of all 4×4 pure density operators, which is diffeomorphic to the complex projective space $\mathbb{CP}^3$.

Furthermore, in this case, the ***concurrence*** C [15], which is commonly used in quantifying entanglement, can be defined as

$$C = 2|\alpha\delta - \beta\gamma| \tag{6.34}$$

(see Appendix B).

Meanwhile, from the equations (C.4) to (C.19) in Appendix C, we have

$$\begin{aligned} |\alpha\delta - \beta\gamma|^2 &= |\alpha|^2|\delta|^2 + \alpha\beta^*\gamma^*\delta - \alpha^*\beta\gamma\delta^* + |\beta|^2|\gamma|^2 \\ &= \frac{1}{8}\left[(\rho_0{}^2 + \widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2) - (\rho_1{}^2 + \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2)\right]. \end{aligned}$$

Then, by the equation (F2) and (C.23) in Appendix C, namely

$$\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2 = \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2, \tag{6.35}$$

and the normalisation condition $\rho_0 = 1$,

$$\begin{aligned} |\alpha\delta - \beta\gamma|^2 &= \frac{1}{4}\left[1 - (\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2)\right] \\ &= \frac{1}{4}\left[1 - (\widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2)\right]. \end{aligned}$$

Consequently we have

$$\mathcal{C} = \sqrt{1 - (\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2)} = \sqrt{1 - (\widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2)}. \tag{6.36}$$

Note that, since every ρ_A is real for the two-qubit pure states, $\mathcal{C}$ varies over the range

$$0 \leq \mathcal{C} \leq 1. \tag{6.37}$$

Remark. From Proposition 2.3, we see that

$$\mathcal{C} = 0 \iff \rho \text{ is separable} \tag{6.38}$$

$$0 < \mathcal{C} \leq 1 \iff \rho \text{ is entangled.} \tag{6.39}$$

In particular, ρ is said to be ***maximally entangled*** if $\mathcal{C} = 1$.

Furthermore the equations (6.36) imply that ρ *is separable if and only if*

$$\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2 = \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 = 1. \tag{6.40}$$

6.2 Reduced density operators

Definition 6.1. Suppose that we have a physical composite system with subsystems S and T, whose state is described by a density operator ρ^{ST}. The ***reduced density operator*** for system S is defined by

$$\rho^S \equiv tr_T(\rho^{ST}), \tag{6.41}$$

where tr_T is a map of operators known as the *partial trace* over system T. The partial trace is defined by

$$tr_T(|s_1\rangle\langle s_2| \otimes |t_1\rangle\langle t_2|) \equiv |s_1\rangle\langle s_2|\, tr(|t_1\rangle\langle t_2|) = |s_1\rangle\langle s_2|\langle t_2|t_1\rangle, \tag{6.42}$$

where s_1 and s_2 are any two vectors in the state space of S, and t_1 and t_2 are any two vectors in the state space of T.

Now we introduce the general definition of a separable pure state (compare Definition 2.4) and a related proposition.

Definition 6.2. Let $\mathcal{E}$ be a state space of a physical composite system with subsystems S and T. A *pure* state $|\psi\rangle \in \mathcal{E}$ for the composite system is said to be ***separable*** if there exist vectors $|\psi_S\rangle \in \mathcal{E}_S$ and $|\psi_T\rangle \in \mathcal{E}_T$ such that

$$|\psi\rangle = |\psi_S\rangle \otimes |\psi_T\rangle, \tag{6.43}$$

where $\mathcal{E}_S$ and $\mathcal{E}_T$ are the state space of subsystems S and T, respectively. Otherwise, the pure state $|\psi\rangle$ is said to be ***entangled***.

Proposition 6.2. *Let $\mathcal{E}$ be a state space of a physical composite system with subsystems S and T, and let $\mathcal{E}_S$ and $\mathcal{E}_T$ be the state spaces of subsystems S and T, respectively. Also let ρ be a pure density operator for the composite system, and let ρ^S and ρ^T be the reduced density operators for subsystems S and T, respectively. If ρ is in a separable state, then*

$$\rho = \rho^S \otimes \rho^T. \tag{6.44}$$

Proof. First note that, since ρ is pure, there exists a state vector $|\psi\rangle \in \mathcal{E}$ such that $\rho = |\psi\rangle\langle\psi|$. Then suppose that ρ is in a separable state, that is, $|\psi\rangle$ is a separable state. Therefore, by definition, there exist vectors $|\psi_S\rangle \in \mathcal{E}_S$ and $|\psi_T\rangle \in \mathcal{E}_T$ such that $|\psi\rangle = |\psi_S\rangle \otimes |\psi_T\rangle$. Thus

$$\rho = (|\psi_S\rangle \otimes |\psi_T\rangle)\,(\langle\psi_S| \otimes \langle\psi_T|) = |\psi_S\rangle\langle\psi_S| \otimes |\psi_T\rangle\langle\psi_T|. \tag{6.45}$$

Here the normalisation condition $\langle\psi|\psi\rangle = 1$ leads to

$$1 = (\langle\psi_S| \otimes \langle\psi_T|)\,(|\psi_S\rangle \otimes |\psi_T\rangle) = \langle\psi_S|\psi_S\rangle\langle\psi_T|\psi_T\rangle. \tag{6.46}$$

Then the reduced density operators ρ^S and ρ^T are

$$\rho^S = tr\,(|\psi_T\rangle\langle\psi_T|)\,|\psi_S\rangle\langle\psi_S| = \langle\psi_T|\psi_T\rangle|\psi_S\rangle\langle\psi_S|,$$

and

$$\rho^T = tr\,(|\psi_S\rangle\langle\psi_S|)\,|\psi_T\rangle\langle\psi_T| = \langle\psi_S|\psi_S\rangle|\psi_T\rangle\langle\psi_T|,$$

respectively. Hence, from (6.45) and (6.46),

$$\begin{aligned}
\rho^S \otimes \rho^T &= (\langle\psi_T|\psi_T\rangle|\psi_S\rangle\langle\psi_S|)\,(\langle\psi_S|\psi_S\rangle|\psi_T\rangle\langle\psi_T|) \\
&= \langle\psi_S|\psi_S\rangle\langle\psi_T|\psi_T\rangle\,(|\psi_S\rangle\langle\psi_S| \otimes |\psi_T\rangle\langle\psi_T|) \\
&= \rho.
\end{aligned}$$

□

In addition, it turns out that, on system S, for any measurement operator $\hat{M}_m$ and the probability $p(m)$ for the outcome m,

$$p(m) = tr(\hat{M}_m{}^\dagger \hat{M}_m \rho^S) = tr\left((\hat{M}_m{}^\dagger \hat{M}_m \otimes I)\rho^{ST}\right), \tag{6.47}$$

and, by the same token, on system T, for any measurement operator $\hat{N}_n$ and the probability $p(n)$ for the outcome n,

$$p(n) = tr(\hat{N}_n{}^\dagger \hat{N}_n \rho^T) = tr\left((I \otimes \hat{N}_n{}^\dagger \hat{N}_n)\rho^{ST}\right). \tag{6.48}$$

(See [16] for more details.)

Now we apply the above properties to our two-qubit pure state case. Recall that a state vector $|\psi\rangle = \alpha|00\rangle+\beta|01\rangle+\gamma|10\rangle+\delta|11\rangle$, where $\alpha, \beta, \gamma, \delta \in \mathbb{C}$, and the corresponding pure density operator $\rho = |\psi\rangle\langle\psi|$ describe the composite system of, say, S and T, whose state space is $\mathcal{E}_S \otimes \mathcal{E}_T$. Then, by applying the partial trace tr_T over system T, the reduced density operator ρ^S for system S is obtained as

$$\begin{aligned}
\rho^S &= tr_T(\rho) = tr_T(|\psi\rangle\langle\psi|) \\
&= tr_T\left[(\alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle)\right. \\
&\qquad \left.\times (\alpha^*\langle 00| + \beta^*\langle 01| + \gamma^*\langle 10| + \delta^*\langle 11|)\right] \\
&= \left(|\alpha|^2 + |\beta|^2\right)|0\rangle\langle 0| + (\alpha\gamma^* + \beta\delta^*)\,|0\rangle\langle 1| \\
&\qquad + (\alpha^*\gamma + \beta^*\delta)\,|1\rangle\langle 0| + \left(|\gamma|^2 + |\delta|^2\right)|1\rangle\langle 1| \\
&= \frac{1}{2}\begin{pmatrix} 1+\rho_1 & -\widetilde{\rho} - i\widetilde{\rho}_1 \\ -\widetilde{\rho} + i\widetilde{\rho}_1 & 1-\rho_1 \end{pmatrix},
\end{aligned} \tag{6.49}$$

where the last line is obtained by the $\{\rho_A\}$-coordinate expressions (6.17) to (6.32). Note that this matrix is in a notably similar form to the density operators ρ for single qubit generic states (compare the equation (5.6)), and, therefore, it is easy to see that $tr(\rho^S) = 1$ and ρ^S is positive, by changing (6.49) into a similar form to (5.6). In fact, like ρ in (5.6), ρ^S belongs to the vector space, say $H_S(2, \mathbb{C})$, of all 2×2 Hermitian operators, which is naturally identified with the subspace

$$span\{I, \widetilde{\Gamma}, \widetilde{\Gamma}_1, \Gamma_1\} = span\{I \otimes I, (-\sigma_1) \otimes I, \sigma_2 \otimes I, \sigma_3 \otimes I\} \tag{6.50}$$

of $H(4, \mathbb{C})$.

In addition, the 'mixedness' $\mathcal{M}(\rho^S)$, which is defined by (5.11), of the reduced density operator ρ^S, is

$$\mathcal{M}(\rho^S) = 2\sqrt{det(\rho^S)} = \sqrt{1 - (\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2)}. \tag{6.51}$$

However, surprisingly, from the equation (6.36), we see that

$$\mathcal{M}(\rho^S) = \mathcal{C}. \tag{6.52}$$

This means that the partial trace operation tr_T over system T maps the manifold $\mathcal{Q}_4$, which consists of all 4×4 pure density operators, onto the closed Bloch 'ball' $\overline{B}_1^3$ (*i.e.* the closure of the open Bloch 'ball' B_1^3) in the subspace $H_S(2, \mathbb{C})$ of $H(4, \mathbb{C})$, namely,

$$tr_T : \begin{array}{ccccc} H(4,\mathbb{C}) \supset & \mathcal{Q}_4(\cong \mathbb{CP}^3) & \longrightarrow & \overline{B}_1^3 & \subset H_S(2,\mathbb{C}) \\ & \rho = |\psi\rangle\langle\psi| & \longmapsto & \rho^S & \end{array}. \tag{6.53}$$

Note that $\overline{B}_1^3$ is, in $H_S(2,\mathbb{C})$, represented by $\rho_0 = 1$ and $\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2 \leq 1$. In addition, we may call it the *first* Bloch 'ball' since it belongs to $H_S(2,\mathbb{C})$ which corresponds to the *first* subsystem S.

Furthermore, under the map tr_T, the set of all the pure density operators with a certain fixed value of the concurrence $\mathcal{C}$ is mapped onto the subset consisting of all the reduced density operators with the fixed 'mixedness' $\mathcal{M}(\rho^S)$ $(= \mathcal{C})$. This forms a concentric spherical shell of the radius $\sqrt{1-\mathcal{C}^2} = \sqrt{1-(\mathcal{M}(\rho^S))^2}$. In particular, the set of all separable density operators (*i.e.* $\mathcal{C} = 0$), is mapped onto the boundary S^2 of $\overline{B}_1^3$, and the set of the maximally entangled density operators (*i.e.* $\mathcal{C} = 1$) goes to the centre of $\overline{B}_1^3$.

Similarly the reduced density operator ρ^T for subsystem T becomes

$$\rho^T = \frac{1}{2}\begin{pmatrix} 1-\widetilde{\rho}_{14} & -\widetilde{\rho}_{12} - i\widetilde{\rho}_{13} \\ -\widetilde{\rho}_{12} + i\widetilde{\rho}_{13} & 1+\widetilde{\rho}_{14} \end{pmatrix}, \tag{6.54}$$

which is a positive operator with a unit trace, and belongs to the subspace

$$\begin{aligned} H_T(2,\mathbb{C}) &\cong span\{I, \widetilde{\Gamma}_{12}, \widetilde{\Gamma}_{13}, \widetilde{\Gamma}_{14}\} \\ &= span\{I\otimes I, I\otimes(-\sigma_1), I\otimes\sigma_2, I\otimes(-\sigma_3)\} \end{aligned} \tag{6.55}$$

of $H(4,\mathbb{C})$. Then the 'mixedness' $\mathcal{M}(\rho^T)$ of ρ^T is

$$\mathcal{M}(\rho^T) = 2\sqrt{det(\rho^T)} = \sqrt{1-(\widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2)}, \tag{6.56}$$

so that, also, $\mathcal{M}(\rho^T) = \mathcal{C}$. Furthermore we see that, by the partial trace operation tr_S over system S, $\mathcal{Q}_4$ is mapped onto the *second* closed Bloch 'ball' $\overline{B}_2^3$: $\rho_0 = 1$ and $\widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 \leq 1$, in the subspace $H_T(2,\mathbb{C})$, that is,

$$tr_S : \begin{array}{ccc} H(4,\mathbb{C}) \supset \ \mathcal{Q}_4(\cong \mathbb{CP}^3) & \longrightarrow & \overline{B}_2^3 \ \subset H_T(2,\mathbb{C}) \\ \rho = |\psi\rangle\langle\psi| & \longmapsto & \rho^T \end{array}. \tag{6.57}$$

Furthermore, just like tr_T, a pure density operator ρ with the concurrence $\mathcal{C}$ is mapped to the reduced density operator ρ^T, whose 'mixedness' is $\mathcal{M}(\rho^T) = \mathcal{C}$, and which is located in the spherical shell of the radius $\sqrt{1-\mathcal{C}^2} = \sqrt{1-(\mathcal{M}(\rho^T))^2}$.

An obvious consequence of the above discussion is the following:

Proposition 6.3. *Let ρ be a 4×4 pure density operator for the composite system of subsystems S and T, and let ρ^S and ρ^T be the reduced density operators for subsystems S and T, respectively. Then, ρ is in a separable state if and only if ρ^S and ρ^T are in pure states.*

Proof. This is obvious from the fact that $\mathcal{C} = \mathcal{M}(\rho^S) = \mathcal{M}(\rho^T)$. $\square$

Remark. The above discussion and the equation (6.40) imply that the set of all separable pure states is the submanifold $S^2 \times S^2$ of $\mathbb{CP}^3$, where $S^2 \times S^2$ is the Cartesian product of the first and second Bloch spheres.

6.3 EPR paradox revisited

Now we return to the "EPR paradox" to see what is actually going on in the EPR thought experiment in terms of our Clifford algebra description.

Recall that the first and second qubits are in the possessions of Alice and Bob, respectively, and the two qubits are in the entangled state

$$|\mathcal{B}\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right), \tag{6.58}$$

so that the corresponding pure density operator is

$$\rho_{\mathcal{B}} = |\mathcal{B}\rangle\langle\mathcal{B}| = \frac{1}{2} \left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11| \right). \tag{6.59}$$

Therefore, by our $\{\rho_A\}$-coordinates (6.17) to (6.32), we have $\rho_0 = \widetilde{\rho}_{34} = 1$ and $\rho_3 = \widetilde{\rho}_4 = -1$, with the other ρ_A being zero. Then, since $\rho_{\mathcal{B}} = \frac{1}{4}\sum_J \rho_J \Gamma_J$,

$$\rho_{\mathcal{B}} = \frac{1}{4} \left(I - \Gamma_3 + \widetilde{\Gamma}_{34} - \widetilde{\Gamma}_4 \right). \tag{6.60}$$

Now let us look back at the equation (6.47), namely

$$p(m) = tr(\hat{M}_m{}^\dagger \hat{M}_m \rho^S) = tr \left((\hat{M}_m{}^\dagger \hat{M}_m \otimes I)\rho^{ST} \right).$$

By the definition (4.1) of $\langle \ , \ \rangle_C$, for this example, the above equation can be rewritten as

$$p(m) = 2 \left\langle \hat{M}_m{}^\dagger \hat{M}_m, \rho_{\mathcal{B}}{}^S \right\rangle_C = 4 \left\langle \hat{M}_m{}^\dagger \hat{M}_m \otimes I, \rho_{\mathcal{B}} \right\rangle_C. \tag{6.61}$$

Significantly this equation implies that the probability $p(m)$ is obtained by working out either the inner product $\langle \hat{M}_m{}^\dagger \hat{M}_m, \rho_{\mathcal{B}}{}^S \rangle_C$ on the Hilbert space $H_S(2, \mathbb{C})$ for subsystem S or the inner product $\langle \hat{M}_m{}^\dagger \hat{M}_m \otimes I, \rho_{\mathcal{B}} \rangle_C$ on the Hilbert space $H(4, \mathbb{C})$ for the composite system of S and T. Obviously it is easier to deal with the former case, so that we now work out the reduced density operator $\rho_{\mathcal{B}}{}^S$.

From the equation (6.49) and (6.54), we have

$$\rho_B{}^S = \rho_B{}^T = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{6.62}$$

Note that, in this case, we have $\mathcal{C} = \mathcal{M}(\rho_B{}^S) = \mathcal{M}(\rho_B{}^T) = 1$, and this shows that ρ_B is maximally entangled. Therefore, $\rho_B{}^S$ and $\rho_B{}^T$ are maximally mixed, and located at the centre of the first Bloch 'ball' $\overline{B}_1^3$ and the second Bloch 'ball' $\overline{B}_2^3$, respectively.

Let us remember that Alice's measurement operators are

$$\{M_m\}_{m=0,1} = \{|m\rangle\langle m| \otimes I\}_{m=0,1}.$$

Now put $\hat{M}_m \equiv |m\rangle\langle m|$, where $m = 0$ or 1, so that we have

$$\hat{M}_m{}^\dagger \hat{M}_m = |m\rangle\langle m|m\rangle\langle m| = |m\rangle\langle m|, \qquad \text{where } m = 0 \text{ or } 1.$$

Note that $\{M_m\}_{m=0,1}$ become measurement operators on Alice's subsystem S since

$$M_0{}^\dagger M_0 + M_1{}^\dagger M_1 = |0\rangle\langle 0| + |1\rangle\langle 1| = I.$$

Then, by the equation (6.47),

$$\begin{aligned} p(m) &= tr(M_m{}^\dagger M_m \rho_B) = tr(\hat{M}_m{}^\dagger \hat{M}_m \rho_B{}^S) \\ &= \frac{1}{2} tr(|m\rangle\langle m|) = \frac{1}{2}\langle m|m\rangle = \frac{1}{2}. \end{aligned}$$

where $m = 0$ or 1. As seen before, this means that Alice obtains either outcome 0 or 1 at 50% probability.

In the same way, Bob's measurement operators are

$$\{N_n\}_{n=0,1} = \{I \otimes |n\rangle\langle n|\}_{n=0,1} = \{I \otimes \hat{N}_n\}_{n=0,1},$$

where $\hat{N}_n \equiv |n\rangle\langle n|$ and $n = 0$ or 1. Then, similarly, we have $\hat{N}_n{}^\dagger \hat{N}_n = |n\rangle\langle n|$, which are measurement operators on Bob's subsystem T, and

$$\begin{aligned} p(n) &= tr(N_n{}^\dagger N_n \rho_B) = tr(\hat{N}_n{}^\dagger \hat{N}_n \rho_B{}^T) \\ &= \frac{1}{2} tr(|n\rangle\langle n|) = \frac{1}{2}. \end{aligned}$$

where $n = 0$ or 1, so that Bob also has an equal 50% chance to obtain each outcome.

However, as we have seen in Chapter 2, the story becomes totally different if Alice first makes a measurement immediately followed by Bob's measurement. Recall that, if Alice obtains the outcome 0, then the new density operator becomes $\rho_B' = |00\rangle\langle 00|$, so that, from the $\{\rho_A\}$-coordinates (6.17) to (6.32), we have $\rho_0 = \rho_1 = 1$ and $\widetilde{\rho}_{14} = \widetilde{\rho}_4 = -1$, with the other ρ_A being zero. Thus

$$\rho_B' = |00\rangle\langle 00| = \frac{1}{4}\left(I + \Gamma_1 - \widetilde{\Gamma}_{14} - \widetilde{\Gamma}_4\right). \tag{6.63}$$

Furthermore, from the equations (6.49) and (6.54), the new reduced density operators ${\rho_B}^{S'}$ and ${\rho_B}^{T'}$ are:

$${\rho_B}^{S'} = {\rho_B}^{T'} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 0|. \tag{6.64}$$

Note that the fact that $\mathcal{C} = \mathcal{M}({\rho_B}^{S'}) = \mathcal{M}({\rho_B}^{T'}) = 0$ indicates that ρ_B' is non-entangled, and ${\rho_B}^{S'}$ and ${\rho_B}^{T'}$ are on the boundary of their respective Bloch balls, namely the first and second Bloch sphere.

Then the probability $p'(0)$ for the outcome 0 is:

$$\begin{aligned} p'(0) &= tr({N_0}^{\dagger} N_0 \rho_B') = tr({\hat{N}_0}^{\dagger} \hat{N}_0 {\rho_B}^{T'}) \\ &= tr(|0\rangle\langle 0|0\rangle\langle 0|) = \langle 0|0\rangle\langle 0|0\rangle = 1. \end{aligned}$$

On the other hand, the probability $p'(1)$ for the outcome 1 is:

$$\begin{aligned} p'(1) &= tr({N_1}^{\dagger} N_1 \rho_B') = tr({\hat{N}_1}^{\dagger} \hat{N}_1 {\rho_B}^{T'}) \\ &= tr(|1\rangle\langle 1|0\rangle\langle 0|) = \langle 1|0\rangle\langle 0|1\rangle = 0. \end{aligned}$$

Therefore Bob has the outcome 0 with certainty.

In similar fashion, it can be shown that Bob's outcome becomes 1 with certainty if Alice has the outcome 1.

We now provide a more geometrically precise explanation for this thought experiment. Firstly, let us see how the fact that Alice has an equal 50% probability for each outcome can be explained in terms of our geometrical picture.

Recall that the probability $p(m)$ for the outcome m is obtained by calculating twice the inner product $\langle {\hat{M}_m}^{\dagger} \hat{M}_m, {\rho_B}^S\rangle_C$ in the Hilbert space $H_S(2, \mathbb{C})$, namely

$$p(m) = 2\left\langle {\hat{M}_m}^{\dagger} \hat{M}_m, {\rho_B}^S \right\rangle_C = tr\left({\hat{M}_m}^{\dagger} \hat{M}_m {\rho_B}^S\right) = \frac{1}{2}.$$

Now remember that, in this case,

$$\rho_{\mathcal{B}}{}^{S} = \frac{1}{2}I \quad \text{and} \quad \hat{M}_m{}^{\dagger}\hat{M}_m = |m\rangle\langle m|, \qquad \text{where } m\text{=0 or 1.}$$

Then, as a basis for Alice's Hilbert space $H_S(2,\mathbb{C})$, let us choose the set $\{I, \check{\Gamma}, \check{\Gamma}_1, \hat{\Gamma}_1\}$, where $\check{\Gamma} \equiv -\sigma_1$, $\check{\Gamma}_1 \equiv \sigma_2$ and $\hat{\Gamma}_1 = i\check{\Gamma}\check{\Gamma}_1 \equiv \sigma_3$ (compare (6.50) and Example 3.3). Therefore, using this basis, we have

$$\begin{aligned}
\rho_{\mathcal{B}}{}^{S} &= \frac{1}{2}I, \\
\hat{M}_0{}^{\dagger}\hat{M}_0 &= |0\rangle\langle 0| = \frac{1}{2}(I + \hat{\Gamma}_1), \\
\hat{M}_1{}^{\dagger}\hat{M}_1 &= |1\rangle\langle 1| = \frac{1}{2}(I - \hat{\Gamma}_1).
\end{aligned}$$

Then, we see that the probability $p(m)$ can be also calculated in terms of $\{\rho_A\}$-coordinates as shown in the equation (4.6):

$$\begin{aligned}
p(0) &= 2\left\langle \hat{M}_0{}^{\dagger}\hat{M}_0, \rho_{\mathcal{B}}{}^{S}\right\rangle_C = \frac{1}{2}\left\langle I + \hat{\Gamma}_1, I\right\rangle_C \\
&= \frac{1}{2}(1 \times 1 + 1 \times 0) = \frac{1}{2},
\end{aligned}$$

and

$$\begin{aligned}
p(1) &= 2\left\langle \hat{M}_1{}^{\dagger}\hat{M}_1, \rho_{\mathcal{B}}{}^{S}\right\rangle_C = \frac{1}{2}\left\langle I - \hat{\Gamma}_1, I\right\rangle_C \\
&= \frac{1}{2}(1 \times 1 - 1 \times 0) = \frac{1}{2}.
\end{aligned}$$

Now let us see what is going on by drawing a diagram (see Figure 1). Despite the fact that $\hat{M}_m{}^{\dagger}\hat{M}_m$ and $\rho_{\mathcal{B}}{}^{S}$ are vectors in the 4-dimensional Hilbert space $H_S(2,\mathbb{C})$, it is sufficient to focus on its subspace $span\{I, \hat{\Gamma}_1\}$ (or the $\rho_0\rho_1$-plane) since $\widetilde{\rho} = \widetilde{\rho}_1 = 0$. In Figure 1, the first Bloch 'ball' $\overline{B}_1^3$ is illustrated as a line segment, while the three vectors $\hat{M}_0{}^{\dagger}\hat{M}_0$, $\hat{M}_1{}^{\dagger}\hat{M}_1$ and $\rho_{\mathcal{B}}{}^{S}$ are also shown. Clearly, from the figure, the inner products $\langle \hat{M}_0{}^{\dagger}\hat{M}_0, \rho_{\mathcal{B}}{}^{S}\rangle_C$ and $\langle \hat{M}_1{}^{\dagger}\hat{M}_1, \rho_{\mathcal{B}}{}^{S}\rangle_C$ are equal, so that the probabilities $p(0)$ and $p(1)$ are also equal.

Now let us turn to Bob's Hilbert space $H_T(2,\mathbb{C})$, and explain, using a similar diagram, why he always obtains the outcome 0 right after Alice found her outcome 0.

We choose the set $\{I, \check{\Gamma}_{12}, \check{\Gamma}_{13}, \check{\Gamma}_{14}\}$, where $\check{\Gamma}_{12} \equiv -\sigma_1$, $\check{\Gamma}_{13} \equiv \sigma_2$ and $\check{\Gamma}_{14} \equiv i\check{\Gamma}_{12}\check{\Gamma}_{13} = \sigma_3$, as a basis for Bob's Hilbert space $H_T(2,\mathbb{C})$ (compare

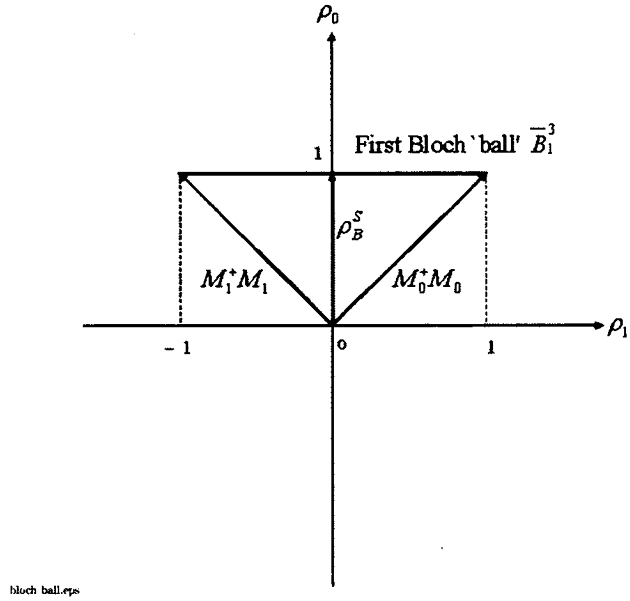

Figure 1: This diagram shows the $\rho_0\rho_1$-plane in Alice's Hilbert space $H_S(2,\mathbb{C})$. In the plane, the first Bloch 'ball' $\overline{B}_1^3$ is represented as the line segment between the points $(-1,1)$ and $(1,1)$, whereas the operators $\hat{M}_0{}^\dagger\hat{M}_0$, $\hat{M}_1{}^\dagger\hat{M}_1$ and $\rho_B{}^S$ are illustrated as vectors.

(6.55) and Example 3.3). Then we have

$$
\begin{aligned}
\rho_B{}^{T'} &= |0\rangle\langle 0| = \frac{1}{2}(I+\check{\Gamma}_{14}),\\
\hat{N}_0{}^\dagger\hat{N}_0 &= |0\rangle\langle 0| = \frac{1}{2}(I+\check{\Gamma}_{14}),\\
\hat{N}_1{}^\dagger\hat{N}_1 &= |1\rangle\langle 1| = \frac{1}{2}(I-\check{\Gamma}_{14}).
\end{aligned}
$$

Therefore the probability for each outcome is:

$$
\begin{aligned}
p'(0) &= 2\left\langle \hat{N}_0{}^\dagger\hat{N}_0, \rho_B{}^{T'}\right\rangle_C = \frac{1}{2}\left\langle I+\check{\Gamma}_{14}, I+\check{\Gamma}_{14}\right\rangle_C\\
&= \frac{1}{2}(1\times 1+1\times 1) = 1,
\end{aligned}
$$

and

$$
\begin{aligned}
p'(1) &= 2\left\langle \hat{N}_1{}^\dagger\hat{N}_1, \rho_B{}^{T'}\right\rangle_C = \frac{1}{2}\left\langle I+\check{\Gamma}_{14}, I-\check{\Gamma}_{14}\right\rangle_C\\
&= \frac{1}{2}(1\times 1+1\times(-1)) = 0.
\end{aligned}
$$

Geometrically, this is explained as follows (see Figure 2). Analogously to Alice's case, we need to consider only the subspace $span\{I,\check{\Gamma}_{14}\}$ (or $\rho_0\widetilde{\rho}_{14}$-plane) of $H_T(2,\mathbb{C})$ since $\widetilde{\rho}_{12}=\widetilde{\rho}_{13}=0$. As its counterpart on $H_S(2,\mathbb{C})$, the second Bloch 'ball' $\overline{B}_2^3$ is drawn as a line segment, and the vectors $\hat{N}_0{}^\dagger\hat{N}_0$,

$\hat{N}_1{}^\dagger \hat{N}_1$ and $\rho_B{}^{T'}$ are shown in Figure 2. Clearly, the fact that $\rho_B{}^{T'} = \hat{N}_0{}^\dagger \hat{N}_0$ indicates that

$$p'(0) = 2\left\langle \hat{N}_0{}^\dagger \hat{N}_0, \rho_B{}^{T'} \right\rangle_C = 2\left\| \rho_B{}^{T'} \right\|_C^2 = 2 \times \frac{1}{2} = 1,$$

where the equation (4.23) is applied, while the picture shows that $\rho_B{}^{T'}$ and $\hat{N}_1{}^\dagger \hat{N}_1$ are orthogonal, so that

$$p'(1) = 2\left\langle \hat{N}_1{}^\dagger \hat{N}_1, \rho_B{}^{T'} \right\rangle_C = 0.$$

Then the question is "Why was Bob's reduced density operator changed into $\rho_B{}^{T'}$ as a consequence of the measurement done by Alice who is far apart from Bob?". The answer of this question may be given as follows.

Alice's reduced density operator was originally in the maximally mixed state $\rho_B{}^S$, which corresponds to the maximally entangled state ρ_B for the composite system (*i.e.* $\mathcal{C} = \mathcal{M}(\rho_B{}^S) = 1$). Then, right after her measurement, her reduced density operator changed into the pure state $\rho_B{}^{S'}$, which corresponds to the separable state $\rho_B{}'$ (*i.e.* $\mathcal{C} = \mathcal{M}(\rho_B{}^{S'}) = 0$). However, because of the correlation equation between the concurrence and the mixednesses, namely

$$\mathcal{C} = \mathcal{M}(\rho_B{}^{S'}) = \mathcal{M}(\rho_B{}^{T'}), \tag{6.65}$$

the state of Bob's reduced density operator *must* be changed into a pure state. In other words, Bob's reduced density operator was forced to relocate from the centre of the second Bloch 'ball' $\overline{B}_2^3$ to its boundary, that is, the second Bloch sphere.

In similar fashion, the other phenomena of the "EPR paradox" can be satisfactorily explained in terms of our geometrical description based on Clifford algebra.

However we must emphasise that, unlike the EPR example, if Alice's and Bob's qubits are in a separable pure state, a measurement done by one of them does not affect the other's measurement outcome. We give a reason for this fact as a closing remark.

Suppose that their qubits are in a separable pure state described by a density operator ρ. From Proposition 6.2, we see that $\rho = \rho^S \otimes \rho^T$, where ρ^S and ρ^T are the reduced density operators for subsystem S and T, respectively. Note that Proposition 6.3 indicates that ρ^S and ρ^T are in pure states.

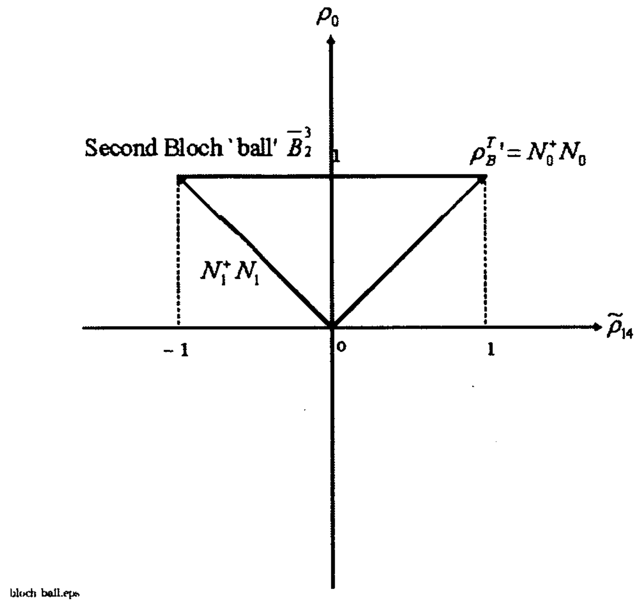

Figure 2: The figure illustrates the $\rho_0\widetilde{\rho}_{14}$-plane in Bob's Hilbert space $H_T(2,\mathbb{C})$. In this plane, the second Bloch 'ball' $\overline{B}_2^3$ is shown as the line segment connecting the points $(-1,1)$ and $(1,1)$, and the operators $\hat{N}_0{}^\dagger\hat{N}_0$, $\hat{N}_1{}^\dagger\hat{N}_1$ and $\rho_B{}^{T'}$ are represented as vectors.

Now suppose that Alice makes a measurement which is described by the measurement operator $M_m = \hat{M}_m \otimes I$, where $m = 0$ or 1, as seen before. Then immediately after her measurement, ρ changes to

$$\begin{aligned}\rho' &= \frac{M_m\rho M_m{}^\dagger}{tr(M_m{}^\dagger M_m\rho)} = \frac{(\hat{M}_m\otimes I)(\rho^S\otimes\rho^T)(\hat{M}_m{}^\dagger\otimes I)}{tr\left((\hat{M}_m{}^\dagger\hat{M}_m\otimes I)(\rho^S\otimes\rho^T)\right)}\\ &= \frac{(\hat{M}_m\rho^S\hat{M}_m{}^\dagger\otimes\rho^T)}{tr(\hat{M}_m{}^\dagger\hat{M}_m\rho^S)tr(\rho^T)} = \frac{(\hat{M}_m\rho^S\hat{M}_m{}^\dagger\otimes\rho^T)}{tr(\hat{M}_m{}^\dagger\hat{M}_m\rho^S)}.\end{aligned}$$

Therefore

$$\rho^{T'} = tr_S(\rho') = \frac{tr(\hat{M}_m\rho^S\hat{M}_m{}^\dagger)}{tr(\hat{M}_m{}^\dagger\hat{M}_m\rho^S)}\rho^T = \rho^T.$$

Hence the probability for the measurement outcome n is

$$p'(n) = tr(\hat{N}_n{}^\dagger\hat{N}_n\rho^{T'}) = tr(\hat{N}_n{}^\dagger\hat{N}_n\rho^T) = p(n).$$

This means that Alice's measurement has no influence upon Bob's measurement outcomes.

7 Conclusion

In this thesis, we have explored the geometrical aspects of quantum states with the help of Clifford algebras.

We introduced the complex Clifford algebra $Cl_N(\mathbb{C})$ and its matrix representation $Mat(D, \mathbb{C})$, where $N = 2n$, $D = 2^n$ and n is an arbitrary natural number, as a platform for our geometrical description of quantum states. We showed that the matrix representation $Mat(D, \mathbb{C})$ is naturally equipped with the Clifford algebra inner product and the Clifford algebra metric, so that $Mat(D, \mathbb{C})$ can be regarded as a Hilbert space and a Riemannian manifold. Furthermore we proved that the space $\mathcal{Q}_D$ of all $D \times D$ pure density operators, which is completely characterised by the Fierz identities and the normalisation condition, can be considered as a smooth manifold, and, in fact, it is diffeomorphic to the complex projective space $\mathbb{CP}^{D-1}$. Moreover the naturally derived fibre bundle projection $S^{2D-1} \to \mathbb{CP}^{D-1}$, which maps a normalised vector $\psi \in S^{2D-1}$ to the corresponding equivalence class $z \in \mathbb{CP}^{D-1}$, provides the natural correspondence between the two formulations of quantum mechanics, namely, the state vector and the density operator formulations.

We provided more concrete discussions on the single qubit and two-qubit cases in terms of our Clifford algebra description. For single qubit states, we defined the 'mixedness' for a generic state, which also plays a vital role in the two-qubit case, and showed that the space $\mathcal{Q}_2$ is identified with $\mathbb{CP}^1$ as a Riemannian manifold. In the case of two-qubit pure states, with the help of the reduced density operators, we explicitly described the geometry of the space $\mathcal{Q}_4$ alongside the Fierz identities. In particular, we showed that the concurrence $\mathcal{C}$ of a two-qubit pure density operator is nothing but the 'mixedness' of the reduced density operator for the subsystem corresponding to each qubit, and it can be explicitly expressed in terms of the $\{\rho_A\}$-coordinates. From this viewpoint, the phenomena of the "EPR paradox" can be explained in a satisfactory manner.

Further investigations

The work presented in this thesis represents only the initial part of an extended investigation of the role of Clifford algebras in the geometry of entanglement. There are several areas in which further work is needed, which could have been pursued if extra time had been available, as well as some more substantial research questions.

Firstly, an obvious extension of our discussion is to describe the geometry of entanglement in n-qubit cases, where $n \geq 3$, in terms of our Clifford algebra formulation. In the higher dimensional cases, the correlation between the concurrence of a two-qubit pure density operator and the 'mixedness' of the reduced density operators could be generalised, and they would play key roles. Then, with the help of this generalisation, phenomena of entanglement such as quantum teleportation (see [16]) could be examined in a similar manner to our "EPR paradox" example.

Secondly, in this thesis we did not examine whether the space $\mathcal{Q}_D$ of all $D \times D$ pure density operators and the complex projective space $\mathbb{CP}^{D-1}$ are identical as Riemannian manifolds apart from in the single qubit case. This should be proved by showing that the metric on $\mathcal{Q}_D$, which is naturally induced from the Clifford algebra metric on $Mat(D, \mathbb{C})$, is nothing but the Fubini-Study metric on $\mathbb{CP}^{D-1}$. (A related discussion for the case of Dirac spinors has been given by Crawford [5].)

Finally, a significant extension of the thesis work would be to relate the Clifford algebra description of the density operators to algebraic geometry. The Fierz identities are a set of homogeneous quadratic equations in D^2 real coordinates, each of whose zero set, as well as the normalisation condition, defines a hypersurface, as shown in section 4.2, and the intersection of all the hypersurfaces turns out to be diffeomorphic to $\mathbb{CP}^{D-1}$. Furthermore the space of all separable pure density operators would be obtained by adding some extra non-Fierz equations as a submanifold of $\mathbb{CP}^{D-1}$. This geometrical hierarchy could be explored from the algebraic geometrical viewpoint. For example, for the two-qubit case, we saw that the space of all separable pure density operators was considered as the submanifold $S^2 \times S^2 \cong \mathbb{CP}^1 \times \mathbb{CP}^1$ of $\mathbb{CP}^3$. This could be explained, from the viewpoint of algebraic geometry, in relation to the Segre embedding (see [19]) in the context of our Clifford algebra formulation. (A related discussion has been given by Życzkowski and Bengtsson [24].)

APPENDIX

A Complex projective spaces $\mathbb{CP}^m$

Throughout this thesis, the complex projective spaces $\mathbb{CP}^m$ play a crucial role. Thus, in this section, we provide the definitions of $\mathbb{CP}^m$ and some of their properties, which characterise $\mathbb{CP}^m$ as Kähler manifolds.

The ***complex projective space*** $\mathbb{CP}^m$ is defined as follows.

For any $(z_1, z_2, \ldots, z_{m+1}), (z'_1, z'_2, \ldots, z'_{m+1}) \in (\mathbb{C}^{m+1})^* \equiv \mathbb{C}^{m+1} \setminus \{0\}$, an equivalence relation $\sim$ is defined as follows.

$$(z_1, z_2, \ldots, z_{m+1}) \sim (z'_1, z'_2, \ldots, z'_{m+1})$$

if there exists $\lambda \in \mathbb{C}^* \equiv \mathbb{C} \setminus \{0\}$ such that

$$z_i = \lambda z'_i \quad \text{for all } i = 1, 2, \ldots, m+1.$$

Then $\mathbb{CP}^m$ is defined by

$$\mathbb{CP}^m \equiv (\mathbb{C}^{m+1})^*/\!\sim\; = \{[z_1 : z_2 : \cdots : z_{m+1}] \mid (z_1, z_2, \ldots, z_{m+1}) \in (\mathbb{C}^{m+1})^*\},$$

where $[z_1 : z_2 : \cdots : z_{m+1}]$ is the equivalence class (called the *homogeneous coordinates*) to which $(z_1, z_2, \ldots, z_{m+1})$ belongs.

Equivalently, $\mathbb{CP}^m$ can be defined in the following way.

For any $(z_1, z_2, \ldots, z_{m+1}), (z'_1, z'_2, \ldots, z'_{m+1}) \in S^{2m+1}$, an equivalence relation $\sim$ is defined as follows.

$$(z_1, z_2, \ldots, z_{m+1}) \sim (z'_1, z'_2, \ldots, z'_{m+1})$$

if there exists $\chi \in [0, 2\pi)$ such that

$$z_i = e^{i\chi} z'_i \quad \text{for all } i = 1, 2, \ldots, m+1.$$

Then $\mathbb{CP}^m$ is defined by

$$\mathbb{CP}^m \cong S^{2m+1}/\!\sim\; = \{[z_1 : z_2 : \cdots : z_{m+1}] \mid (z_1, z_2, \ldots, z_{m+1}) \in S^{2m+1}\}.$$

Note that, since $e^{i\chi} \in S^1 \cong U(1)$,

$$\mathbb{CP}^m \cong S^{2m+1}/S^1 \cong S^{2m+1}/U(1).$$

Then it is easily seen that the above two definitions are equivalent.

Now we give an informal definition of a fibre bundle as follows. A ***fibre bundle*** has five features, namely, the total space E, the base space B, the projection p, the fibre F and the group of bundle G. E, B and F are topological spaces and p is a continuous surjection from E onto B. In addition, for any point x in B, there exists an open neighbourhood U such that $p^{-1}(U) \cong U \times F$. In other words, a fibre bundle is locally homeomorphic to the product topological space $U \times F$, and for each x in B, $p^{-1}(x)$ is homeomorphic to the fibre F. The simplest example of fibre bundles is a product space $B \times F$, which is called a ***trivial*** bundle (see [21] for more details).

The complex projective space $\mathbb{CP}^m$ is naturally equipped with the fibre bundle structure in the following way. The definition of $\mathbb{CP}^m$ naturally induces the map

$$h : \begin{array}{ccc} S^{2m+1} & \longrightarrow & \mathbb{CP}^m \\ (z_1, z_2, \ldots, z_{m+1}) & \longmapsto & [z_1 : z_2 : \cdots : z_{m+1}] \end{array} .$$

Then, regarding the map h as the bundle projection, $S^{2m+1} \longrightarrow \mathbb{CP}^m$ becomes a S^1 fibre bundle. (For more details see, for example, [4] pp.507.)

The complex projective space $\mathbb{CP}^m$ turns out to be an m-dimensional Kähler manifold, which is a complex manifold endowed with a Kähler metric. In fact, the fact that $\mathbb{CP}^m$ is an m-dimensional complex manifold can be shown in the following way.

Theorem A.1. *The complex projective space $\mathbb{CP}^m$ is an m-dimensional complex manifold.*

Proof. Put $z \equiv [z_1 : z_2 : \cdots : z_{m+1}]$ and $U_j \equiv \{z \in \mathbb{CP}^m | z_j \neq 0\}$. Then $z \in U_1$ is represented as

$$z = [1 : \zeta_1^2 : \zeta_1^3 : \cdots : \zeta_1^{m+1}], \quad \text{where } \zeta_1^l = z_l / z_1.$$

Now we consider the map

$$\zeta_1 : \begin{array}{ccc} U_1 & \longrightarrow & \mathbb{C}^m \\ z & \longmapsto & \zeta_1 = (\zeta_1^2, \zeta_1^3, \cdots, \zeta_1^{m+1}) \end{array} .$$

It is easily seen that ζ_1 is a biholomorphism onto $\mathbb{C}^m$, so that it gives local coordinates on U_1. Similarly, on U_j, we define local coordinates

$$\zeta_j : \begin{array}{ccc} U_j & \longrightarrow & \mathbb{C}^m \\ z & \longmapsto & \zeta_j = (\zeta_j^1, \cdots, \zeta_j^{j-1}, \zeta_j^{j+1}, \cdots, \zeta_j^{m+1}) \end{array} ,$$

where $\zeta_j^l = z_l/z_j$. Evidently ζ_j is also biholomorphic. On $U_j \cap U_k$, we have

$$\zeta_j^k = \frac{1}{\zeta_k^j}, \quad \zeta_j^l = \frac{\zeta_k^l}{\zeta_k^j}, \quad \text{where } j \neq k,\ k \neq l \text{ and } l \neq j.$$

Hence the coordinate transformations

$$\zeta_j \circ \zeta_k^{-1}|_{\zeta_k(U_j \cap U_k)} : \begin{array}{ccccccc} \mathbb{C}^m & \supset & \zeta_k(U_j \cap U_k) & \longrightarrow & \zeta_j(U_j \cap U_k) & \subset & \mathbb{C}^m \\ & & \zeta_k(z) & \longmapsto & \zeta_j(z) & & \end{array},$$

where $\zeta_j(z) = (\frac{\zeta_k^1}{\zeta_k^j}, \cdots, \frac{\zeta_k^{j-1}}{\zeta_k^j}, \frac{\zeta_k^{j+1}}{\zeta_k^j}, \cdots, \frac{\zeta_k^{m+1}}{\zeta_k^j})$, are biholomorphic. Therefore $\mathbb{CP}^m$ is considered as a m-dimensional complex manifold obtained by the $(m+1)$-copies of $\mathbb{C}^m$ via the biholomorphisms $\zeta_j \circ \zeta_k^{-1}|_{\zeta_k(U_j \cap U_k)}$. □

The natural Kähler metric on $\mathbb{CP}^m$ is called the ***Fubini-Study metric***. The definition of the Fubini-Study metric on $\mathbb{CP}^m$ is given as follows.

For given two points $[z_1, \dots, z_{m+1}], [z_1 + dz_1, \dots, z_{m+1} + dz_{m+1}] \in \mathbb{CP}^m$, the distance ds between them is

$$ds^2 = 2 \sum_{j,k=1}^{m+1} \frac{z_{[j,}dz_{k]}\, {z^*_{[j,}dz_{k]}}^*}{|z_j|^4}, \tag{A.1}$$

where index commutator notation is used, so that

$$z_{[j,}w_{k]} = \frac{1}{2}(z_j w_k - z_k w_j).$$

(For more details see, for example, [10].)

B Single and two-qubit pure states and the Hopf bundles

In this section, we give a summary of the Hopf bundle description of single qubit and two-qubit pure states, which is presented by Mosseri and Dandoloff [15]. In their formulation, the space of the single qubit pure states is described as the first Hopf bundle $S^3 \to S^2$, and this view precisely agrees with our Clifford algebra description. However, in their case, the space of two-qubit pure states is considered as the second Hopf bundle $S^7 \to S^4$ along with the quaternions, which is quite different from our view.

B.1 Complex projective space $\mathbb{CP}^1$ and the first Hopf bundle

The complex projective space $\mathbb{CP}^1$ is defined in the way which is shown in Appendix A. Furthermore, importantly, we can see that $\mathbb{CP}^1$ is nothing but S^2. To see this, we first prove the following theorem.

Theorem B.1. *The complex projective space $\mathbb{CP}^1$ is identified with the 2-dimensional sphere S^2 as a smooth manifold (i.e. $\mathbb{CP}^1$ is diffeomorphic to S^2), and a diffeomorphism between $\mathbb{CP}^1$ and S^2 may be given by*

$$\pi : \begin{array}{ccc} \mathbb{CP}^1 & \xrightarrow{\cong} & S^2 \\ [z_1 : z_2] & \longmapsto & (x_0, x_1, x_2) \end{array}, \tag{B.1}$$

where $x_0 = 2Re(z_1^* z_2)$, $x_1 = 2Im(z_1^* z_2)$, $x_2 = |z_2|^2 - |z_1|^2$ *and* $|z_1|^2 + |z_2|^2 = 1$.

Proof. To see that the map π is in fact a diffeomorphism, firstly notice that the points (x_0, x_1, x_2) are surely located in S^2 since

$$x_0{}^2 + x_1{}^2 + x_2{}^2 = 4|z_1^* z_2|^2 + \left(|z_2|^2 - |z_1|^2\right)^2 = \left(|z_1|^2 + |z_2|^2\right)^2 = 1.$$

Secondly π does not depend on choice of representative element for each equivalence class $[z_1 : z_2]$. To see this, let us choose $(e^{i\chi} z_1, e^{i\chi} z_2) \in S^3$ as another representative for the equivalence class $[z_1 : z_2]$. In this case, we have

$$(e^{i\chi} z_1)^* (e^{i\chi} z_2) = (e^{-i\chi} z_1^*)(e^{i\chi} z_2) = z_1^* z_2,$$

and

$$|e^{i\chi} z_2|^2 - |e^{i\chi} z_1|^2 = |z_2|^2 - |z_1|^2.$$

This shows that π is independent of choice of (z_1, z_2) and, therefore, well-defined.

Next we show that π is bijective. Now note that

$$\mathbb{CP}^1 \ni [z_1 : z_2] = [z_1 z_1{}^* : z_2 z_1{}^*] = \left[|z_1|^2 : z_1{}^* z_2\right].$$

Thus, for $(x_0, x_1, x_2) \in S^2$, we can always find its inverse image under this map by putting

$$|z_1|^2 = \frac{1 - x_2}{2} \quad \text{and} \quad z_1{}^* z_2 = \frac{x_0 + i x_1}{2}.$$

In this case, z_1 is not uniquely determined but this inverse image does not depend on choice of z_1. To see this, let us choose another candidate $e^{i\chi} z_1$, which satisfies the equation

$$|e^{i\chi} z_1|^2 = \frac{1 - x_2}{2}.$$

This time we are forced to choose $e^{i\chi} z_2$ instead of z_2 since

$$(e^{i\chi} z_1)^* (e^{i\chi} z_2) = z_1^* z_2 = \frac{x_0 + i x_1}{2}.$$

However, we still have the same inverse image of (x_0, x_1, x_2) since

$$\left[e^{i\chi} z_1, e^{i\chi} z_2\right] = [z_1, z_2].$$

This shows that π is bijective.

Lastly, to complete the proof that the map π is a diffeomorphism, we show that both π and π^{-1} are smooth. From Theorem A.1, we see that, in the case of $\mathbb{CP}^1$, two coordinate systems (U_1, ζ_1) and (U_2, ζ_2) can be chosen. If $z \in U_1$, we have the composite map

$$\pi|_{U_1} \circ \zeta_1^{-1} : \begin{array}{ccccc} \mathbb{C} & \xrightarrow{\zeta_1^{-1}} & U_1 & \xrightarrow{\pi|_{U_1}} & S^2 \\ \zeta_1^2 = z_2/z_1 & \longmapsto & z = [z_1 : z_2] & \longmapsto & (x_0, x_1, x_2) \end{array}.$$

Now we put $\zeta \equiv \zeta_1^2$ for simplicity, then

$$x_0 + i x_1 = 2 z_1^* z_2 = \frac{2 z_1^* z_2}{|z_1|^2 + |z_2|^2} = \frac{2\zeta}{|\zeta|^2 + 1},$$

and

$$x_2 = |z_2|^2 - |z_1|^2 = \frac{|z_2|^2 - |z_1|^2}{|z_1|^2 + |z_2|^2} = \frac{|\zeta|^2 - 1}{|\zeta|^2 + 1}.$$

Therefore

$$(x_0, x_1, x_2) = \left(\frac{2Re\zeta}{|\zeta|^2+1}, \frac{2Im\zeta}{|\zeta|^2+1}, \frac{|\zeta|^2-1}{|\zeta|^2+1} \right).$$

This is nothing other than the inverse map of the stereographic projection $\mathbb{C} \longrightarrow S^2 \setminus \{(0,0,1)\}$, and clearly it is smooth [23].

Similarly, if $z \in U_2$, we have

$$\pi|_{U_2} \circ \zeta_2^{-1} : \begin{array}{ccccc} \mathbb{C} & \xrightarrow{\zeta_2^{-1}} & U_2 & \xrightarrow{\pi|_{U_2}} & S^2 \\ \zeta_2^1 = z_1/z_2 & \longmapsto & z = [z_1 : z_2] & \longmapsto & (x_0, x_1, x_2) \end{array}.$$

Then, putting $\xi \equiv \zeta_2^1$, we have

$$x_0 + ix_1 = \frac{2\xi^*}{|\xi|^2+1} \quad \text{and} \quad x_2 = \frac{1-|\xi|^2}{|\xi|^2+1}.$$

Therefore

$$(x_0, x_1, x_2) = \left(\frac{2Re\xi}{|\xi|^2+1}, -\frac{2Im\xi}{|\xi|^2+1}, \frac{1-|\xi|^2}{|\xi|^2+1} \right).$$

This is also the inverse of the stereographic projection $\mathbb{C} \longrightarrow S^2 \setminus \{(0,0,-1)\}$, and it is smooth. Hence the bijection π is a diffeomorphism from $\mathbb{CP}^1$ onto S^2. □

Remark. The point $(e^{i\chi}z_1, e^{i\chi}z_2)$ is on a great circle, which is uniquely determined by each (z_1, z_2), in S^3. In fact, this great circle is nothing but the fibre of each point $[z_1 : z_2]$ in the base space S^2 for the first Hopf bundle, which we will see below.

For $\mathbb{CP}^1$, the Fubini-Study metric defined by (A.1) agrees with the standard round metric on the Bloch sphere (or Riemann sphere) S^2. In fact, for the above coordinate system (U_1, ζ_1), this metric is expressed as

$$ds^2 = \frac{d\zeta d\zeta^*}{(1+|\zeta|^2)^2} = \frac{dx^2+dy^2}{(1+r^2)^2} = d\theta^2 + \sin^2\theta d\varphi^2, \qquad \text{(B.2)}$$

where $\zeta = z_2/z_1 = x + iy$, and $r^2 = \zeta\zeta^* = x^2 + y^2$, while θ, φ are the usual spherical coordinates, given by projecting the sphere down to the complex plane, with $\tan(\theta/2) = r$, $\cos\varphi = x/r$ and $\sin\varphi = y/r$.

Note that, here, if $\theta = 0$, we have $r = 0$, so that φ is not defined. However, in this case, $\theta = 0$ leads to $ds^2 = d\theta^2$, and the metric is safely defined. On the other hand, if $\theta = \pi$, which corresponds to the north pole on S^2, Equation (B.2) does not make sense since the condition $\tan(\theta/2) = r$ is not valid.

Similarly, for the coordinate system (U_2, ζ_2), this metric is denoted as

$$ds^2 = \frac{d\xi d\xi^*}{(1+|\xi|^2)^2} = \frac{dx'^2 + dy'^2}{(1+r'^2)^2} = d\theta'^2 + \sin^2\theta' d\varphi'^2, \tag{B.3}$$

where $\xi = z_1/z_2 = x' + iy'$, $r'^2 = \xi\xi^* = x'^2 + y'^2$, $\tan(\theta'/2) = r'$, $\cos\varphi' = x'/r'$ and $\sin\varphi' = y'/r'$. Note that, similarly to the previous case, if $\theta' = \pi$ (*i.e.* the south pole), Equation (B.3) is invalid.

However, since

$$x' + iy' = \xi = \frac{1}{\zeta} = \frac{1}{x+iy} = \frac{1}{r^2}(x - iy)$$

on $U_1 \cap U_2$, we have

$$x' = \frac{x}{r^2}, \ y' = -\frac{y}{r^2} \ \text{ and } \ r' = \frac{1}{r}.$$

In addition, we have

$$\begin{aligned}
tan\frac{\theta'}{2} &= r' = \frac{1}{r} = \frac{1}{tan(\theta/2)} = tan\left(\frac{\pi}{2} - \frac{\theta}{2}\right), \\
cos\varphi' &= \frac{x'}{r'} = \frac{x}{r^2}r = \frac{x}{r} = cos\varphi = cos(-\varphi), \\
sin\varphi' &= \frac{y'}{r'} = \frac{-y}{r^2}r = -\frac{y}{r} = -sin\varphi = sin(-\varphi).
\end{aligned}$$

This indicates that we can choose a coordinate transformation between (U_1, ζ_1) and (U_2, ζ_2) which satisfies

$$r' = \frac{1}{r}, \ \theta' = \pi - \theta \ \text{ and } \ \varphi' = -\varphi.$$

Then,

$$d\theta' = -d\theta, \ d\varphi' = -d\varphi \ \text{ and } \ sin\theta' = sin(\pi - \theta) = sin\theta$$

lead to

$$d\theta'^2 + sin^2\theta' d\varphi'^2 = (-d\theta)^2 + sin^2\theta(-d\varphi)^2 = d\theta^2 + sin^2\theta d\varphi^2.$$

This shows that (B.2) and (B.3) coincide completely on $U_1 \cap U_2$. Furthermore, if $\theta = \pi$, we have $\theta' = \pi - \pi = 0$, so that the metric can be written as

$$ds^2 = d\theta'^2 = (-d\theta)^2 = d\theta^2.$$

This means that the metric is expressed, entirely on S^2 (*i.e.* $0 \le \theta \le \pi$ and $0 \le \varphi < 2\pi$), as

$$ds^2 = d\theta^2 + \sin^2\theta d\varphi^2.$$

Remark. The above discussion indicates that $\mathbb{CP}^1$ is isometric to S^2, so that they are equivalent as Riemannian manifolds (see the footnote on page 35).

In addition, the definition of $\mathbb{CP}^1$ naturally yields the ***first Hopf map***

$$h: \begin{array}{ccccc} S^3 & \longrightarrow & \mathbb{CP}^1 & \stackrel{\cong}{\longrightarrow} & S^2 \\ (z_1, z_2) & \longmapsto & [z_1 : z_2] & \longmapsto & (x_0, x_1, x_2) \end{array} \tag{B.4}$$

Consequently, we have the ***first Hopf bundle*** with the total space S^3, the base space S^2 and the projection h. It is easy to see that local triviality holds. Indeed, the equation (2.3), namely

$$|\psi\rangle = e^{i\chi}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right), \qquad \chi, \varphi \in [0, 2\pi) \text{ and } \theta \in [0, \pi),$$

implies the local triviality of this fibre bundle.

However, the first Hopf bundle is non-trivial. In fact, we know that, from cohomology theory [23],

$$H^1(S^2 \times S^1) \cong \mathbb{Z} \quad \text{and} \quad H^1(S^3) = 0.$$

On the other hand, if the fibre bundle is trivial (*i.e.* $S^3 \cong S^2 \times S^1$), the fact that cohomology groups are topological invariants leads to

$$H^1(S^2 \times S^1) \cong H^1(S^3),$$

which contradicts the above facts. Therefore the first Hopf bundle can not be trivial.

B.2 Single qubit pure states and the first Hopf bundle

According to Mosseri and Dandoloff [15], the set of single qubit pure states can be identified with ***the first Hopf bundle*** $S^3 \longrightarrow S^2$ as follows.

The ***first Hopf map*** (the projection p of the first Hopf bundle) is, in this case, defined as the composition of a map h_1 from S^3 to $\mathbb{R}^2 \cup \{\infty\}$ and an inverse stereographic map h_2 from $\mathbb{R}^2 \cup \{\infty\}$ to S^2:

$$h_1 \; : \; \begin{array}{ccc} S^3 & \longrightarrow & \mathbb{R}^2 \cup \{\infty\} \\ (\alpha, \beta) & \longmapsto & C = (\alpha\beta^{-1})^* \end{array} \qquad \alpha, \beta \in \mathbb{C} \tag{B.5}$$

$$h_2 \; : \; \begin{array}{ccc} \mathbb{R}^2 \cup \{\infty\} & \longrightarrow & S^2 \\ C & \longmapsto & (X, Y, Z) \end{array} \qquad X^2 + Y^2 + Z^2 = 1, \tag{B.6}$$

where

$$\begin{aligned} X &= \langle\sigma_1\rangle_\psi = \langle\psi|\sigma_1|\psi\rangle = 2Re(\alpha^*\beta), \\ Y &= \langle\sigma_2\rangle_\psi = \langle\psi|\sigma_2|\psi\rangle = 2Im(\alpha^*\beta), \\ Z &= \langle\sigma_3\rangle_\psi = \langle\psi|\sigma_3|\psi\rangle = |\alpha|^2 - |\beta|^2. \end{aligned} \tag{B.7}$$

Note that the map $h_2 \circ h_1$ and its image S^2 are nothing but the canonical projection from S^3 onto the complex projective space $\mathbb{CP}^1 \cong S^2$ and a Bloch sphere, respectively. Furthermore $\{\infty\}$ goes to the north pole $(0, 0, 1)$ of the S^2 by the h_2 map.

In addition, note that for any $|\psi\rangle \in S^3$ and $\chi \in [0, 2\pi]$,

$$(e^{\mathbf{i}\chi}\alpha)^*(e^{\mathbf{i}\chi}\beta) = (e^{-\mathbf{i}\chi}\alpha^*)(e^{\mathbf{i}\chi}\beta) = \alpha^*\beta \qquad \text{and}$$
$$|e^{\mathbf{i}\chi}\alpha|^2 - |e^{\mathbf{i}\chi}\beta|^2 = |\alpha|^2 - |\beta|^2.$$

Hence, both $|\psi\rangle$ and $exp\mathbf{i}\chi|\psi\rangle$ are mapped to the same point (X, Y, Z) in the base space S^2. This shows that our fibre bundle for the single qubit states has the fibre S^1 which is parameterized by χ.

B.3 Quaternions

The quaternions are members of the noncommutative algebra with the fundamental formula $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$, which was invented as analogy to the complex numbers. With the imaginary units $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ and the fundamental above formula, the quaternions are represented in the form

$$q = x_0 + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k} \qquad x_0, x_1, x_2, x_3 \in \mathbb{R}$$

Equivalently, by using the complex numbers $c_1 = x_0 + x_1\mathbf{i}$ and $c_2 = x_2 + x_3\mathbf{i}$, they can also be written in the form $q = c_1 + c_2\mathbf{j}$.

The conjugate $\overline{q}$ of a quaternion q is given by

$$\overline{q} = x_0 - x_1\mathbf{i} - x_2\mathbf{j} - x_3\mathbf{k} = \overline{c_1} - c_2\mathbf{j}.$$

and its norm $|q|$ is defined by

$$|q| = \sqrt{q\overline{q}} = \sqrt{|c_1|^2 + |c_2|^2} = \sqrt{x_0^2 + x_1^2 + x_2^2 + x_3^2}.$$

Therefore, obviously, the equation $|q| = 1$ represents a unit 3-sphere. Also, the inverse q^{-1} of the quaternion q is given by: $q^{-1} = \overline{q}/(q\overline{q})$.

The quaternions are closely related to four vectors. In that sense, a quaternion q can be interpreted as the sum of a scalar part $S(q)$ and a vector part $\mathbf{V}(q)$. That is,

$$q = S(q) + \mathbf{V}(q) \qquad S(q) = x_0 \qquad \mathbf{V}(q) = x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k}.$$

A quaternion is said to be *real* if $\mathbf{V}(q) = 0$, and *purely imaginary* if $S(q) = 0$. In addition, a quaternion can be written in an exponential form as

$$q = |q|exp(\varphi\mathbf{t}) = |q|(\cos\varphi + \mathbf{t}\sin\varphi),$$

where φ is a real number and $\mathbf{t}$ is a unit purely imaginary quaternion. We see that , by letting $\mathbf{t} = \mathbf{i}$, the complex numbers are contained in the quaternions. Note that quaternion multiplication is non-commutative so that

$$exp(\varphi\mathbf{t})exp(\lambda\mathbf{u}) = exp(\varphi\mathbf{t} + \lambda\mathbf{u})$$

only if $\mathbf{t} = \mathbf{u}$.

B.4 Two-qubit pure states and the second Hopf bundle

In the case of two-qubit pure states, the bundle projection (namely the Hopf map) can be defined in the similar manner to the single qubit case as follows. Suppose that

$$q_1 = \alpha + \beta\mathbf{j}, \qquad q_2 = \gamma + \delta\mathbf{j}, \qquad q_1, q_2 \in \mathbb{H}. \tag{B.8}$$

Then, $|q_1|^2+|q_2|^2 = |\alpha|^2+|\beta|^2+|\gamma|^2+|\delta|^2 = 1$ implies that (q_1, q_2) represents a point in S^7. The Hopf map from the total space S^7 to the base S^4 is the composition of a map h_1 from S^7 to $\mathbb{R}^4 \cup \{\infty\}$, and an inverse stereographic map h_2 from $\mathbb{R}^4 \cup \{\infty\}$ to S^4.

$$h_1 \;:\; \begin{array}{ccc} S^7 & \longrightarrow & \mathbb{R}^4 \cup \{\infty\} \\ (q_1, q_2) & \longmapsto & Q = (q_1 q_2^{-1})^* \end{array} \qquad q_1, q_2 \in \mathbb{H}, \tag{B.9}$$

$$h_2 \;:\; \begin{array}{ccc} \mathbb{R}^4 \cup \{\infty\} & \longrightarrow & S^4 \\ Q & \longmapsto & (x_0, x_1, x_2, x_3, x_4) \end{array} \qquad \sum_{l=0}^{4} x_l^2 = 1. \tag{B.10}$$

Similarly to the previous single qubit case, the map h_1 is the canonical projection from S^7 onto the quaternionic projective space $\mathbb{HP}^1$. It is well-known that this fibre bundle (called the ***second Hopf bundle***) is also non-trivial. Furthermore, it can be easily seen that the fibre of the bundle is S^3.

In addition, the above Hopf map has the following coordinate expressions.

$$\begin{aligned}
x_0 &= cos2\Omega = |q_1|^2 - |q_2|^2 = |\alpha|^2 + |\beta|^2 - |\gamma|^2 - |\delta|^2, && \text{(B.11)}\\
x_1 &= sin2\Omega S(Q') = 2Re(\alpha^*\gamma + \beta^*\delta), && \text{(B.12)}\\
x_2 &= sin2\Omega V_{\mathbf{i}}(Q') = 2Im(\alpha^*\gamma + \beta^*\delta), && \text{(B.13)}\\
x_3 &= sin2\Omega V_{\mathbf{j}}(Q') = 2Re(\alpha\delta - \beta\gamma), && \text{(B.14)}\\
x_4 &= sin2\Omega V_{\mathbf{k}}(Q') = 2Im(\alpha\delta - \beta\gamma), && \text{(B.15)}
\end{aligned}$$

where $sin2\Omega = 2|q_1||q_2|$, $Q' = Q/|Q|$ and

$$Q' = S(Q') + \mathbf{V}(Q') = S(Q') + V_{\mathbf{i}}(Q')\mathbf{i} + V_{\mathbf{j}}(Q')\mathbf{j} + V_{\mathbf{k}}(Q')\mathbf{k}$$

with $S(Q'), V_{\mathbf{i}}(Q'), V_{\mathbf{j}}(Q'), V_{\mathbf{k}}(Q') \in \mathbb{R}$.

Remark. Similarly to the single qubit case, the above coordinate expressions can be rewritten by using the Pauli matrices as follows. Firstly, let us define $\mathbf{J}$ as the (antilinear) 'conjugator', an operator which takes the complex conjugate of all complex numbers in an expression (here, $\mathbf{J}$ acts on the left-hand side in the scalar product below). Then, define the antilinear operator $\mathbf{E}$ by: $\mathbf{E} = -\mathbf{J}(\sigma_2 \otimes \sigma_2)$. Now, we see that

$$\begin{aligned}
x_0 &= \langle\sigma_3 \otimes I\rangle_\psi = \langle\psi|\sigma_3 \otimes I|\psi\rangle = |\alpha|^2 + |\beta|^2 - |\gamma|^2 - |\delta|^2,\\
x_1 &= \langle\sigma_1 \otimes I\rangle_\psi = \langle\psi|\sigma_1 \otimes I|\psi\rangle = 2Re(\alpha^*\gamma + \beta^*\delta),\\
x_2 &= \langle\sigma_2 \otimes I\rangle_\psi = \langle\psi|\sigma_2 \otimes I|\psi\rangle = 2Im(\alpha^*\gamma + \beta^*\delta), && \text{(B.16)}\\
x_3 &= Re\langle\mathbf{E}\rangle_\psi = 2Re(\alpha\delta - \beta\gamma),\\
x_4 &= Im\langle\mathbf{E}\rangle_\psi = 2Im(\alpha\delta - \beta\gamma).
\end{aligned}$$

Furthermore, we can define the ***concurrence*** $\mathcal{C}$, which is widely used for quantifying entanglement, in terms of the S^7 description by

$$\mathcal{C} = |\langle\mathbf{E}\rangle_\Psi| = 2|\alpha\delta - \beta\gamma|. \qquad \text{(B.17)}$$

Note that $\mathcal{C}$ varies over the range $0 \leq \mathcal{C} \leq 1$, and $\mathcal{C}$ vanishes for non-entangled states.

Finally, we provide a rough topological picture of the space of two-qubit pure states. Under the Hopf map $h_2 \circ h_1$, the image of all separable states becomes the two dimensional sphere ${x_0}^2 + {x_1}^2 + {x_2}^2 = 1$ in the base space S^4 since $\alpha\delta = \beta\gamma$ (or $\mathcal{C} = 0$) leads to $x_3 = x_4 = 0$. Also, in this case, it turns out that the fibre reduces to S^2. Therefore, the subset of all separable states in the total space S^7 is $S^2 \times S^2$, where each S^2 is the Bloch sphere for each qubit.

On the other hand, all entangled states are mapped onto the complement $S^4 \setminus S^2$ of the Bloch sphere in the base space S^4 by the Hopf map. Then, it can be shown that $S^4 \setminus S^2$ is a disjoint union of circles S^1, and, on each circle, the fibre S^3 reduces to the real projective space $\mathbb{RP}^3 \cong S^3/\mathbb{Z}_2$.

C Fierz identities for two-qubit pure states

In this appendix, we use the identities (I) to (VI) (see Section 6.1), which have been derived by exploiting the condition that ρ has rank 1, as derived in Corollary 4.6, to compute the following 9 Fierz identities for the two-qubit case. At the end of the appendix, a sample calculation is given as a comparison, of a Fierz identity for the product ${\rho_0}^2$ coming directly from the method of equation (4.16).

(F1) ${\rho_0}^2 = {\rho_1}^2 + {\rho_2}^2 + {\rho_3}^2 + {\rho_4}^2 + \widetilde{\rho}^2$

(F2) ${\rho_0}^2 = {\widetilde{\rho}_1}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_3}^2 + {\widetilde{\rho}_4}^2 + \widetilde{\rho}^2$

(F3) ${\rho_0}^2 = {\rho_2}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{14}}^2 + {\widetilde{\rho}_{34}}^2$

(F4) $\rho_0\rho_1 + \widetilde{\rho}_{13}\widetilde{\rho}_3 = \widetilde{\rho}_{12}\widetilde{\rho}_2 + \widetilde{\rho}_{14}\widetilde{\rho}_4$

(F5) $\rho_0\widetilde{\rho}_4 = \rho_1\widetilde{\rho}_{14} + \rho_2\widetilde{\rho}_{24} + \rho_3\widetilde{\rho}_{34}$

(F6) $\rho_2\rho_3 = \widetilde{\rho}_{12}\widetilde{\rho}_3 + \widetilde{\rho}_{13}\widetilde{\rho}_2 + \widetilde{\rho}_{24}\widetilde{\rho}_{34}$

(F7) $\rho_3\widetilde{\rho}_{24} = \rho_2\widetilde{\rho}_{34} + \rho_4\widetilde{\rho}_{23} + \widetilde{\rho}_1\widetilde{\rho}$

(F8) $\rho_0\widetilde{\rho} + \rho_1\widetilde{\rho} + \widetilde{\rho}_{14}\widetilde{\rho} + \widetilde{\rho}_4\widetilde{\rho} + \rho_2\widetilde{\rho}_3 + \widetilde{\rho}_{24}\widetilde{\rho}_3 = \rho_0\widetilde{\rho}_{23} + \rho_1\widetilde{\rho}_{23}$
$+ \widetilde{\rho}_{14}\widetilde{\rho}_{23} + \widetilde{\rho}_4\widetilde{\rho}_{23} + \rho_2\widetilde{\rho}_{13} + \rho_3\widetilde{\rho}_{12} + \rho_3\widetilde{\rho}_2 + \widetilde{\rho}_{34}\widetilde{\rho}_2 + \widetilde{\rho}_{12}\widetilde{\rho}_{34} + \widetilde{\rho}_{13}\widetilde{\rho}_{24}$

(F9) $\rho_3\widetilde{\rho}_{13} + \widetilde{\rho}_{13}\widetilde{\rho}_{34} = \rho_0\rho_4 + \rho_0\widetilde{\rho}_1 + \rho_1\rho_4 + \rho_1\widetilde{\rho}_1 + \rho_4\widetilde{\rho}_{14} + \rho_4\widetilde{\rho}_4$
$+ \widetilde{\rho}_{14}\widetilde{\rho}_1 + \widetilde{\rho}_1\widetilde{\rho}_4 + \rho_2\widetilde{\rho}_{12} + \rho_2\widetilde{\rho}_2 + \rho_3\widetilde{\rho}_{34} + \rho_3\widetilde{\rho}_3 + \widetilde{\rho}_{12}\widetilde{\rho}_{24} + \widetilde{\rho}_{24}\widetilde{\rho}_2.$

To see how we obtain the above 9 identities, firstly note that we have the following identities for complex numbers α, β, γ and δ:

$$\begin{aligned} & |\alpha^*\gamma - \beta^*\delta|^2 + |\alpha^*\beta + \gamma^*\delta|^2 \\ = \; & |\alpha^*\gamma + \beta^*\delta|^2 + |\alpha^*\beta - \gamma^*\delta|^2 \\ = \; & \left(|\alpha|^2 + |\delta|^2\right)\left(|\beta|^2 + |\gamma|^2\right), \end{aligned} \tag{C.1}$$

$$\begin{aligned} & |\alpha^*\beta - \gamma\delta^*|^2 + |\alpha^*\delta + \beta^*\gamma|^2 \\ = \; & |\alpha^*\beta + \gamma\delta^*|^2 + |\alpha^*\delta - \beta^*\gamma|^2 \\ = \; & \left(|\alpha|^2 + |\gamma|^2\right)\left(|\beta|^2 + |\delta|^2\right), \end{aligned} \tag{C.2}$$

$$\begin{aligned} & |\alpha^*\delta - \beta\gamma^*|^2 + |\alpha^*\gamma + \beta\delta^*|^2 \\ = \; & |\alpha^*\delta + \beta\gamma^*|^2 + |\alpha^*\gamma - \beta\delta^*|^2 \\ = \; & \left(|\alpha|^2 + |\beta|^2\right)\left(|\gamma|^2 + |\delta|^2\right). \end{aligned} \tag{C.3}$$

Meanwhile, from the $\{\rho_A\}$-coordinates (6.17) to (6.32), we have

$$
\begin{aligned}
4|\alpha|^2 &= \rho_0 + \rho_1 - \widetilde{\rho}_{14} - \widetilde{\rho}_4, &\quad (C.4)\\
4|\beta|^2 &= \rho_0 + \rho_1 + \widetilde{\rho}_{14} + \widetilde{\rho}_4, &\quad (C.5)\\
4|\gamma|^2 &= \rho_0 - \rho_1 - \widetilde{\rho}_{14} + \widetilde{\rho}_4, &\quad (C.6)\\
4|\delta|^2 &= \rho_0 - \rho_1 + \widetilde{\rho}_{14} - \widetilde{\rho}_4, &\quad (C.7)\\
4\alpha^*\beta &= (-\widetilde{\rho}_{12} - \widetilde{\rho}_2) + i(\widetilde{\rho}_{13} - \widetilde{\rho}_3), &\quad (C.8)\\
4\alpha\beta^* &= (-\widetilde{\rho}_{12} - \widetilde{\rho}_2) - i(\widetilde{\rho}_{13} - \widetilde{\rho}_3), &\quad (C.9)\\
4\gamma^*\delta &= (-\widetilde{\rho}_{12} + \widetilde{\rho}_2) + i(\widetilde{\rho}_{13} + \widetilde{\rho}_3), &\quad (C.10)\\
4\gamma\delta^* &= (-\widetilde{\rho}_{12} + \widetilde{\rho}_2) - i(\widetilde{\rho}_{13} + \widetilde{\rho}_3), &\quad (C.11)\\
4\alpha^*\gamma &= (-\widetilde{\rho} + \widetilde{\rho}_{23}) + i(\widetilde{\rho}_1 + \rho_4), &\quad (C.12)\\
4\alpha\gamma^* &= (-\widetilde{\rho} + \widetilde{\rho}_{23}) - i(\widetilde{\rho}_1 + \rho_4), &\quad (C.13)\\
4\beta^*\delta &= (-\widetilde{\rho} - \widetilde{\rho}_{23}) + i(\widetilde{\rho}_1 - \rho_4), &\quad (C.14)\\
4\beta\delta^* &= (-\widetilde{\rho} - \widetilde{\rho}_{23}) - i(\widetilde{\rho}_1 - \rho_4), &\quad (C.15)\\
4\alpha^*\delta &= (\widetilde{\rho}_{34} - \rho_3) + i(\rho_2 - \widetilde{\rho}_{24}), &\quad (C.16)\\
4\alpha\delta^* &= (\widetilde{\rho}_{34} - \rho_3) - i(\rho_2 - \widetilde{\rho}_{24}), &\quad (C.17)\\
4\beta^*\gamma &= (\widetilde{\rho}_{34} + \rho_3) + i(\rho_2 + \widetilde{\rho}_{24}), &\quad (C.18)\\
4\beta\gamma^* &= (\widetilde{\rho}_{34} + \rho_3) - i(\rho_2 + \widetilde{\rho}_{24}). &\quad (C.19)
\end{aligned}
$$

Then, by substituting some of the equations (C.4) to (C.19) into the equations (C.1), (C.2) and (C.3), we have

$$
\begin{aligned}
{\rho_0}^2 - {\widetilde{\rho}_4}^2 &= {\rho_4}^2 + {\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{23}}^2\\
&= {\widetilde{\rho}_1}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_3}^2 + \widetilde{\rho}^2, \qquad (C.20)
\end{aligned}
$$

$$
\begin{aligned}
{\rho_0}^2 - {\widetilde{\rho}_{14}}^2 &= {\rho_2}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{34}}^2 + {\widetilde{\rho}_2}^2\\
&= {\rho_3}^2 + {\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_3}^2, \qquad (C.21)
\end{aligned}
$$

$$
\begin{aligned}
{\rho_0}^2 - {\rho_1}^2 &= {\rho_2}^2 + {\rho_3}^2 + {\rho_4}^2 + \widetilde{\rho}^2\\
&= {\widetilde{\rho}_{23}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_{34}}^2 + {\widetilde{\rho}_1}^2. \qquad (C.22)
\end{aligned}
$$

Alternative forms of these equations may be

$$
\begin{aligned}
{\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{14}}^2 &= \widetilde{\rho}^2 + {\widetilde{\rho}_1}^2 + {\rho_1}^2, &\quad (C.23)\\
{\widetilde{\rho}_{14}}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_3}^2 &= {\rho_1}^2 + {\widetilde{\rho}_{23}}^2 + {\rho_4}^2, &\quad (C.24)\\
{\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_3}^2 + {\widetilde{\rho}_4}^2 &= {\rho_1}^2 + {\rho_2}^2 + {\widetilde{\rho}_{34}}^2, &\quad (C.25)\\
{\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_4}^2 &= {\rho_1}^2 + {\rho_3}^2 + {\widetilde{\rho}_{24}}^2, &\quad (C.26)\\
{\widetilde{\rho}_{14}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_{34}}^2 &= {\rho_4}^2 + {\widetilde{\rho}_4}^2 + \widetilde{\rho}^2, &\quad (C.27)\\
{\widetilde{\rho}_{23}}^2 + {\widetilde{\rho}_1}^2 + {\widetilde{\rho}_4}^2 &= {\rho_2}^2 + {\rho_3}^2 + {\widetilde{\rho}_{14}}^2. &\quad (C.28)
\end{aligned}
$$

Now we turn to the identities (I) to (VI) on page 49, namely,

(I) $\left(|\alpha|^2\right)\left(|\beta|^2\right) = (\alpha^*\beta)(\alpha\beta^*)$

(II) $\left(|\beta|^2\right)\left(|\gamma|^2\right) = (\beta^*\gamma)(\beta\gamma^*)$

(III) $\left(|\gamma|^2\right)\left(|\delta|^2\right) = (\gamma^*\delta)(\gamma\delta^*)$

(IV) $(\alpha^*\beta)(\gamma^*\delta) = (\alpha^*\delta)(\beta\gamma^*)$

(V) $(\alpha^*\gamma)(\beta^*\delta) = (\alpha^*\delta)(\beta^*\gamma)$

(VI) $(\alpha^*\beta)(\beta^*\gamma) = \left(|\beta|^2\right)(\alpha^*\gamma)$.

Firstly we substitute the equations (C.4), (C.5), (C.8) and (C.9) into (I). Then we have

$$\left(\widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 - \rho_0{}^2 - \rho_1{}^2\right) + 2\left(\widetilde{\rho}_2\widetilde{\rho}_{12} - \widetilde{\rho}_3\widetilde{\rho}_{13} + \widetilde{\rho}_4\widetilde{\rho}_{14} - \rho_0\rho_1\right) = 0. \tag{C.29}$$

Similarly, from (III), the following equation is obtained:

$$\left(\widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 - \rho_0{}^2 - \rho_1{}^2\right) - 2\left(\widetilde{\rho}_2\widetilde{\rho}_{12} - \widetilde{\rho}_3\widetilde{\rho}_{13} + \widetilde{\rho}_4\widetilde{\rho}_{14} - \rho_0\rho_1\right) = 0. \tag{C.30}$$

By adding the equations (C.29) and (C.30), we have

$$\rho_0{}^2 + \rho_1{}^2 = \widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2. \tag{C.31}$$

Furthermore, by substituting (C.23) into (C.31), we obtain

$$\rho_0{}^2 = \widetilde{\rho}_1{}^2 + \widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}^2, \tag{C.32}$$

which is one of our Fierz identities (F2).

On the other hand, by subtracting (C.30) from (C.29), we obtain

$$\rho_0\rho_1 + \widetilde{\rho}_{13}\widetilde{\rho}_3 = \widetilde{\rho}_{12}\widetilde{\rho}_2 + \widetilde{\rho}_{14}\widetilde{\rho}_4, \tag{C.33}$$

which is the Fierz identity (F4).

Next, by rewriting the equation (II) with the $\{\rho_A\}$-coordinates in a similar manner, we have

$$\left(\rho_0{}^2 + \widetilde{\rho}_4{}^2 - \rho_1{}^2 - \rho_2{}^2 - \rho_3{}^2 - \widetilde{\rho}_{14}{}^2 - \widetilde{\rho}_{24}{}^2 - \widetilde{\rho}_{34}{}^2\right) + 2\left(\rho_0\widetilde{\rho}_4 - \rho_1\widetilde{\rho}_{14} - \rho_2\widetilde{\rho}_{24} - \rho_3\widetilde{\rho}_{34}\right) = 0. \tag{C.34}$$

However, from the equation (C.22) and, then, (C.27),

$$\begin{aligned} & \rho_0{}^2 + \widetilde{\rho}_4{}^2 - \rho_1{}^2 - \rho_2{}^2 - \rho_3{}^2 - \widetilde{\rho}_{14}{}^2 - \widetilde{\rho}_{24}{}^2 - \widetilde{\rho}_{34}{}^2 \\ = \; & \rho_4{}^2 + \widetilde{\rho}_4{}^2 - \widetilde{\rho}^2 - \widetilde{\rho}_{14}{}^2 - \widetilde{\rho}_{24}{}^2 - \widetilde{\rho}_{34}{}^2 = 0. \end{aligned}$$

Hence (C.34) reduces to the Fierz identity (F5):

$$\rho_0\widetilde{\rho}_4 = \rho_1\widetilde{\rho}_{14} + \rho_2\widetilde{\rho}_{24} + \rho_3\widetilde{\rho}_{34}. \tag{C.35}$$

We now look at the equation (IV) to transform it by the $\{\rho_A\}$-coordinates. The equation changes into

$$\begin{aligned}\left({\rho_3}^2 + {\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_3}^2 - {\rho_2}^2 - {\widetilde{\rho}_{13}}^2 - {\widetilde{\rho}_{34}}^2 - {\widetilde{\rho}_2}^2\right)& \\ +2i\left(\widetilde{\rho}_2\widetilde{\rho}_{13} + \widetilde{\rho}_3\widetilde{\rho}_{12} + \widetilde{\rho}_{24}\widetilde{\rho}_{34} - \rho_2\rho_3\right) = 0.&\end{aligned} \tag{C.36}$$

Then, since every ρ_A is real in the two-qubit pure state case (see Proposition 3.2), the following two identities are satisfied:

$${\rho_3}^2 + {\widetilde{\rho}_{12}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_3}^2 = {\rho_2}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{34}}^2 + {\widetilde{\rho}_2}^2, \tag{C.37}$$

$$\rho_2\rho_3 = \widetilde{\rho}_2\widetilde{\rho}_{13} + \widetilde{\rho}_3\widetilde{\rho}_{12} + \widetilde{\rho}_{24}\widetilde{\rho}_{34}. \tag{C.38}$$

By substituting the equation (C.2) into (C.37), it can be rewritten as

$${\rho_0}^2 = {\rho_2}^2 + {\widetilde{\rho}_2}^2 + {\widetilde{\rho}_{13}}^2 + {\widetilde{\rho}_{14}}^2 + {\widetilde{\rho}_{34}}^2. \tag{C.39}$$

Then we see that the equation (C.39) and (C.38) are nothing other than the identities (F3) and (F6), respectively.

Now we focus on the identity (V). Similarly to the previous cases, we rewrite it with the $\{\rho_A\}$-coordinates, so that we have

$$\begin{aligned}\left({\rho_2}^2 + {\rho_3}^2 + {\rho_4}^2 + \widetilde{\rho}^2 - {\widetilde{\rho}_{23}}^2 - {\widetilde{\rho}_{24}}^2 - {\widetilde{\rho}_{34}}^2 - {\widetilde{\rho}_1}^2\right)& \\ +2i\left(\rho_3\widetilde{\rho}_{24} - \rho_2\widetilde{\rho}_{34} - \rho_4\widetilde{\rho}_{23} - \widetilde{\rho}_1\widetilde{\rho}\right) = 0.&\end{aligned} \tag{C.40}$$

Then the following two identities are derived from this equation:

$${\rho_2}^2 + {\rho_3}^2 + {\rho_4}^2 + \widetilde{\rho}^2 = {\widetilde{\rho}_{23}}^2 + {\widetilde{\rho}_{24}}^2 + {\widetilde{\rho}_{34}}^2 + {\widetilde{\rho}_1}^2, \tag{C.41}$$

$$\rho_3\widetilde{\rho}_{24} = \rho_2\widetilde{\rho}_{34} + \rho_4\widetilde{\rho}_{23} + \widetilde{\rho}_1\widetilde{\rho}. \tag{C.42}$$

The identity (C.42) is nothing but (F7), and, by substituting the equation (C.3) into (C.41), we have (F1), namely

$${\rho_0}^2 = {\rho_1}^2 + {\rho_2}^2 + {\rho_3}^2 + {\rho_4}^2 + \widetilde{\rho}^2. \tag{C.43}$$

Lastly we substitute some of the $\{\rho_A\}$-coordinate expressions into (VI), and obtain

$$\begin{aligned}&(\rho_0\widetilde{\rho} + \rho_1\widetilde{\rho} + \widetilde{\rho}_{14}\widetilde{\rho} + \widetilde{\rho}_4\widetilde{\rho} + \rho_2\widetilde{\rho}_3 + \widetilde{\rho}_{24}\widetilde{\rho}_3 \\ &-\rho_0\widetilde{\rho}_{23} - \rho_1\widetilde{\rho}_{23} - \widetilde{\rho}_{14}\widetilde{\rho}_{23} - \widetilde{\rho}_4\widetilde{\rho}_{23} - \rho_2\widetilde{\rho}_{13} \\ &-\rho_3\widetilde{\rho}_{12} - \rho_3\widetilde{\rho}_2 - \widetilde{\rho}_{34}\widetilde{\rho}_2 - \widetilde{\rho}_{12}\widetilde{\rho}_{34} - \widetilde{\rho}_{13}\widetilde{\rho}_{24}) \\ &\quad +2i\,(\rho_3\widetilde{\rho}_{13} + \widetilde{\rho}_{13}\widetilde{\rho}_{34} - \rho_0\rho_4 - \rho_0\widetilde{\rho}_1 - \rho_1\rho_4 \\ &\quad -\rho_1\widetilde{\rho}_1 - \rho_4\widetilde{\rho}_{14} - \rho_4\widetilde{\rho}_4 - \widetilde{\rho}_{14}\widetilde{\rho}_1 - \widetilde{\rho}_1\widetilde{\rho}_4 - \rho_2\widetilde{\rho}_{12} \\ &\quad -\rho_2\widetilde{\rho}_2 - \rho_3\widetilde{\rho}_{34} - \rho_3\widetilde{\rho}_3 - \widetilde{\rho}_{12}\widetilde{\rho}_{24} - \widetilde{\rho}_{24}\widetilde{\rho}_2) = 0.\end{aligned} \tag{C.44}$$

Then this identity leads to

$$\begin{aligned}
&\rho_0\widetilde{\rho} + \rho_1\widetilde{\rho} + \widetilde{\rho}_{14}\widetilde{\rho} + \widetilde{\rho}_4\widetilde{\rho} + \rho_2\widetilde{\rho}_3 + \widetilde{\rho}_{24}\widetilde{\rho}_3 \\
&\quad = \rho_0\widetilde{\rho}_{23} + \rho_1\widetilde{\rho}_{23} + \widetilde{\rho}_{14}\widetilde{\rho}_{23} + \widetilde{\rho}_4\widetilde{\rho}_{23} + \rho_2\widetilde{\rho}_{13} \\
&\qquad + \rho_3\widetilde{\rho}_{12} + \rho_3\widetilde{\rho}_2 + \widetilde{\rho}_{34}\widetilde{\rho}_2 + \widetilde{\rho}_{12}\widetilde{\rho}_{34} + \widetilde{\rho}_{13}\widetilde{\rho}_{24},
\end{aligned} \tag{C.45}$$

and

$$\begin{aligned}
\rho_3\widetilde{\rho}_{13} + \widetilde{\rho}_{13}\widetilde{\rho}_{34} &= \rho_0\rho_4 + \rho_0\widetilde{\rho}_1 + \rho_1\rho_4 + \rho_1\widetilde{\rho}_1 + \rho_4\widetilde{\rho}_{14} \\
&\quad + \rho_4\widetilde{\rho}_4 + \widetilde{\rho}_{14}\widetilde{\rho}_1 + \widetilde{\rho}_1\widetilde{\rho}_4 + \rho_2\widetilde{\rho}_{12} + \rho_2\widetilde{\rho}_2 \\
&\qquad + \rho_3\widetilde{\rho}_{34} + \rho_3\widetilde{\rho}_3 + \widetilde{\rho}_{12}\widetilde{\rho}_{24} + \widetilde{\rho}_{24}\widetilde{\rho}_2,
\end{aligned} \tag{C.46}$$

which are (F8) and (F9), respectively.

In relation to the direct identification of the quadratic Fierz identities via methods of Theorem 4.4, it should be noted that a complete enumeration in the current notation is unrealistic, since there are, in principle, 16^4 C_{IJKL}'s (albeit with many interrelationships).

However, to demonstrate the completeness of the set (F1)–(F9), let us substitute for example the values $I = 0$, $J = 0$ in (4.16) (see also (4.10), (6.1)–(6.16)):

$$\rho_0{}^2 = \frac{1}{4}\sum_{K,L} C_{0K0L}\,\rho_K\rho_L,$$

where

$$C_{0K0L} = \frac{1}{4}tr(\Gamma_0\Gamma_K\Gamma_0\Gamma_L).$$

However, since $\Gamma_0 = I$ and (4.1),

$$C_{0K0L} = \frac{1}{4}tr(\Gamma_K\Gamma_L) = G_{KL} = \delta_{KL}.$$

This leads to the following 16-term Fierz identity,

$$\rho_0{}^2 = \frac{1}{4}\sum_K \rho_K{}^2. \tag{C.47}$$

Finally, note that this identity is derivable from (F1) and (F2), with the help of Equations (C.22) and (C.23), as follows:
by adding up the equations

$$\begin{aligned}
\rho_0{}^2 &= \rho_1{}^2 + \rho_2{}^2 + \rho_3{}^2 + \rho_4{}^2 + \widetilde{\rho}^2 \\
\rho_0{}^2 &= \widetilde{\rho}_1{}^2 + \widetilde{\rho}_2{}^2 + \widetilde{\rho}_3{}^2 + \widetilde{\rho}_4{}^2 + \widetilde{\rho}^2 \\
\rho_0{}^2 - \rho_1{}^2 - \widetilde{\rho}_1{}^2 &= \widetilde{\rho}_{23}{}^2 + \widetilde{\rho}_{24}{}^2 + \widetilde{\rho}_{34}{}^2 \\
\widetilde{\rho}^2 + \widetilde{\rho}_1{}^2 + \rho_1{}^2 &= \widetilde{\rho}_{12}{}^2 + \widetilde{\rho}_{13}{}^2 + \widetilde{\rho}_{14}{}^2 \\
\rho_0{}^2 &= \rho_0{}^2,
\end{aligned}$$

we have

$$4{\rho_0}^2 = \sum_K {\rho_K}^2,$$

which is equivalent to equation (C.47).

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